CONTINUOUS vs DISCRETE PROCESSES: THE PROBABILISTIC EVOLUTION OF SINGLE TRAPPED IONS.

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Abstract

The evolution of a single trapped ion exhibiting intermittent fluorescence and dark periods may be described either as a continuous process, using differential rate equations, or discretely, as a Markov process. The latter models the atom as making instantaneous transitions from one energy eigenstate to another, and is open to the objection that superpositions of energy states will form which are not covered by the Markov process. The superposition objection is replied to, and two new mathematical elements, Markov vectors and Markov matrices, are proposed as additions to quantum theory. The paper concludes by attributing the cause of dark periods in the ion's history to instantaneous transitions in the ion itself, rather than to photon detection or other components of measurement.

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References

1. Introduction: shelving and dark periods.

In 1975 Hans Dehmelt, investigating methods of determining the frequency of atomic line emissions to a very high standard of accuracy, suggested that an extremely narrow line-width would be obtained if a single trapped ion's electron were driven to a metastable energy level, and in Dehmelt's suggestive word "shelved" there.

Ten years later, Cook and Kimble (1985) proposed that the concept of shelving could be used to investigate a problem of theoretical interest: the existence of "quantum jumps". A three-level atom in the "V" configuration (Cook and Kimble's figure 1, p. 1023) exhibits resonance fluorescence when irradiated by laser light of the appropriate frequency. The rapid oscillations between levels 1 and 3 give the appearance of constant radiation intensity. But when the weak transition is also stimulated the atom has a small probability of moving to level 2: when this happens the fluorescence is switched off and the atom enters a dark period.

Cook and Kimble noted that, whereas the detection of a single photon emitted by the weak transition is problematic, the beginning and ending of dark periods in the fluorescence is detectable by the human eye aided by a 10X magnifying glass. Their suggestion was therefore that dark periods could provide a means of directly observing the instantaneous atomic transitions that had been the cause of much discussion between Bohr, Heisenberg and Schrödinger.

2. Rate equations for atomic change of state.

The three-level system in the V configuration evolves according to differential equations which govern changes in its density matrix (Kimble, Cook and Wells (1986), p. 3191). The authors show that the system is reducible to a two-level system, the first level consisting of a combination of levels 1 and 3 when fluorescence is occurring and the electron is oscillating back and forth. The second level is the "shelved" state 2.

Where A ("light") and B ("dark") are the levels of the new two-level system, g is the transition rate from A to B, h that from B to A, $P_{\mathrm{A}}(t)$ is the probability of the system being "light" and $P_{\mathrm{B}}(t)$ that of being "dark", the evolution of the fluorescing atom is described by the following simple rate equations:

$$\frac{dP_{\mathrm{A}}}{dt} = -gP_{\mathrm{A}}(t) + hP_{\mathrm{B}}(t); \qquad \frac{dP_{\mathrm{B}}}{dt} = +gP_{\mathrm{A}}(t) - hP_{\mathrm{B}}(t) \tag{1}$$

Solution of these simultaneous equations, starting from initial conditions $P_{\mathrm{A}}(0) = 1$, $P_{\mathrm{B}}(0) = 0$, yields P_{A} and P_{B} as explicit functions of t:

$$P_{\mathrm{A}}(t) = \frac{h + g\,e^{-(g+h)t}}{g+h}; \qquad P_{\mathrm{B}}(t) = \frac{g\left(1 - e^{-(g+h)t}\right)}{g+h} \tag{2}$$

$P_A(t)$ starts at 1 and decays asymptotically to $\dfrac{h}{g+h}$.

$P_B(t)$ starts at 0 and increases asymptotically to $\dfrac{g}{g+h}$.

At all times, $P_A(t) + P_B(t) = 1$.

These rate equations, as well as the density-matrix equations, describe change of state in the fluorescing atom as a smooth, continuous process. The same holds for Itano's rate equations for the evolution of a three-level system in the lambda configuration (levels 1, 2, and 3/4 (=0) of fig. 1 of Itano, Bergquist and Wineland (1988), p. 559). Where γ_1, γ_2 and γ_0 are the decay rates of the levels 1, 2 and 0, and f_1 and f_2 (= $1 - f_1$) give the branching ratio for the transition from level 1 to levels 0 and 2 respectively, the three-level equations (p. 560) are:

$$\frac{dP_1}{dt} = -\gamma_1 P_1 + \gamma_0 P_0 \,; \qquad \frac{dP_2}{dt} = f_2\gamma_1 P_1 - \gamma_2 P_2 \,; \qquad \frac{dP_0}{dt} = f_1\gamma_1 P_1 + \gamma_2 P_2 - \gamma_0 P_0 \tag{3}$$

3. <u>Discrete, non-continuous atomic evolution.</u>

The evolution of the two-level system described by equations (1) and (2), and of the three-level system described by equations (3), is continuous throughout. Nothing in these equations gives any hint of discrete transitions from one state to another, or of the sudden appearance and disappearance of dark periods. Although the rate equations provide answers to questions such as "What is the probability that the system is in a dark period at time *t*?", they cannot answer questions like "What is the probability that a dark period begins at *t* and ends at t' ?" To address questions of this kind, a mathematical description of the atom's evolution is needed which is not based on differential equations, but introduces instantaneous stochastic changes. These changes, though unpredictable, are subject to strict probabilistic constraints, hence are not arbitrary or "chance".

The need for a stochastic approach is recognized in Cook and Kimble (1985) and in Kimble, Cook and Wells (1986). They note that the rate equations (1) do not describe the discrete alternation between light and dark periods of figure 2 of (1985, p. 1023). Their solution is to "adopt a point of view in which time is coarse-grained over intervals which are long compared with $1/A_1$, but short compared with $1/A_2$", where $1/A_1$ and $1/A_2$ are the residence times in levels 1 and 2 respectively (1986, p. 3190). This procedure "converts the temporal variations of the strong fluorescence into a classical stochastic process", so that the atomic fluorescence "resembles a classical random telegraph signal".

4. Sequences of atomic transitions as a Markov process.

Let $\{S_1, S_2, \ldots S_m\}$ be a set of states, which in the case of an atom will be its energy levels, and imagine the atom's optical electron successively occupying these states over a sequence of short time intervals Δt_1, Δt_2, ... of equal duration. At each interval the atom undergoes a change of state or transition (it being understood that the transition may be from a state S_i to itself), and each possible transition is assigned a probability. A Markov process differs from a Bernoulli or Poisson process in that in a Markov process the probability of the transition $S_i \rightarrow S_j$ in or at the end of interval Δt_n depends upon the state S_i of the system in the interval. A system undergoing a Markov process has a "memory", but the memory extends only to its current state, not to the atom's previous history.

Once the division of time into intervals of constant length Δt is established, the properties of the atomic Markov process are summed up in its transition matrix. An example for a two-level process such as the light/dark alternation of a two-level atomic system is the following (Matrix M):

		From:	
		A	B
To:	A	1/2	1/3
	B	1/2	2/3

(4)

When the system corresponding to Matrix M has run for a while, it settles down into a steady state in which the probabilities of finding it in states A and B are 2/5 and 3/5 respectively. Using matrix multiplication, we have that

$$\begin{bmatrix} \frac{1}{2} & \frac{1}{3} \\ \frac{1}{2} & \frac{2}{3} \end{bmatrix} \begin{bmatrix} \frac{2}{5} \\ \frac{3}{5} \end{bmatrix} = \begin{bmatrix} \frac{2}{5} \\ \frac{3}{5} \end{bmatrix},$$

which is to say that (2/5, 3/5) is the eigenvector of the transition matrix M with eigenvalue 1. We return to this topic in section 7 below.

5. Transition matrix for the V configuration.

As an artificial example, consider a fluorescent ion in the V configuration of figure 1 of Cook and Kimble (1985). Let the decay rate of the strong transition $1 \rightarrow 3$ be 1 per ms, corresponding to a natural lifetime of 1 ms, and let the rate for the weak transition $2 \rightarrow 3$ be 0.125 per ms, corresponding to a lifetime of 8 ms. We choose for the purposes of this example $\Delta t = 4$ ms, which accords with Kimble, Cook and Wells' proposal to make time coarse-grained over intervals long compared to the strong dwell-time but short compared to the weak dwell-time. Where γ is the decay rate, both transitions are subject to the law of exponential decay:

$$\text{p(non-decay by time } t) = \exp(-\gamma\, t).$$

We arrive at the following transition matrix:

$$\begin{array}{cccc} & 1 & 2 & 3 \\ 1 & .018 & 0 & .999 \\ 2 & 0 & .607 & .001 \\ 3 & .982 & .393 & 0 \end{array} \tag{5}$$

This matrix describes the behaviour of the three-level ion when time is divided into intervals of 4 ms. It can be used e.g. to calculate the probability that the ion will enter a dark period at time interval Δt_{25} and remain in it until Δt_{40}, at which time the fluorescence recommences.

What remains to be proved concerning the Markov description of atomic processes is that the probabilities of such things as the future occurrence of dark periods of given lengths are stable over different choices of Δt. Thus, for $\Delta t = .04$ ms, the probability value for the dark period from Δt_{2500} to Δt_{4000} should be closely related to the earlier value for Δt_{25} to Δt_{40}. In the limit, the most accurate probability predictions would presumably result from Markov processes based on very short time intervals, possibly of the order of 10^{-40} sec.

6. The superposition objection.

Although the representation of atomic transitions as Markov processes appears to capture the sudden appearance and disappearance of dark periods, there is a powerful objection to the idea that the history of an atom can be written as the successive occupancy of discrete states, with instantaneous transitions in between. The objection is that quantum mechanics permits, and on occasion requires, the atom to enter into a coherent superposition of discrete energy states (see for example Schenzle and Brewer (1986), p. 3128). If the atom is in a linear combination of such states, with complex coefficients, how can it be conceived to jump? Cook ((1990), p. 365) asserts that the formation of coherent superpositions of states in effect "eliminates the quantum-jump picture as a useful interpretation of quantum behaviour".

This objection is a serious one, but it can be answered. Even if the temporal evolution of the atom carries it into a superposition of energy states it can still make discontinuous transitions, and an elegant method of calculating the probabilities for it to jump in different ways can be constructed. This method rests on the addition, in quantum theory, of "Markov vectors" and "Markov matrices" to the traditional categories of vectors and operators in Hilbert space.

7. Markov vectors and Markov matrices.

A normalized vector is a vector of unit length; a "Markov" vector is a vector the components of which are real non-negative numbers which sum to unity, e.g. (1/2, 1/3, 1/6). A vector may be a Markov vector relative to one basis but not to another: e.g. (1, 0) is not a Markov vector when written in a different basis as $(1/\sqrt{2}, 1/\sqrt{2})$.

To any normalized vector $v = (c_1, c_2, \ldots)$ there corresponds a Markov vector
$v+ = (c_1c_1^*, c_2c_2^*, \ldots)$, where c^* is the complex conjugate of c. Since v is normalized,
$c_1c_1^* + c_2c_2^* + \ldots = 1$.

A Markov matrix is a square matrix, each column of which is a Markov vector. Thus the transition matrices (4) and (5) above are Markov matrices, relative to a basis. It is not difficult to generalize the argument in section 4 to show that the product of a Markov matrix and a Markov vector is always a Markov vector, and we conjecture that every Markov matrix has, in the set of Markov vectors, a unique eigenvector with eigenvalue 1, and no eigenvector with eigenvalue other than 1.

8. Resolution of the superposition problem.

In this section we show that superpositions of atomic energy states can be incorporated into Markov processes. Consider an arbitrary linear combination

$$v = a_1u_1 + a_2u_2 + ...$$

where $| v | = 1$ and the basis vectors u_1, u_2, ... are chosen so that each represents one of the atom's discrete energy levels. These energy-vectors are orthogonal. What the vector v represents is an atomic state with a complex amplitude a_1 of being at energy level u_1, an amplitude a_2 of being at level u_2, ... etc. The Markov vector

$$v+ = a_1a_1{}^*u_1 + a_2a_2{}^*u_2 + ...$$

yields $a_1a_1{}^*$ as the probability of an atom in state $|v\rangle$ being in state $|u_1\rangle$, $a_2a_2{}^*$ as the probability of being in state $|u_2\rangle$, etc.

To show that atomic transitions of an atom in an arbitrary superposition of energy states can be dealt with using Markov methods, consider for simplicity a two-level case. Let S be an atomic system with energy levels A and B, let $u_1 = (1, 0)$ represent the state A, and let $u_2 = (0, 1)$ represent B. Suppose that the Markov matrix M of section 4 above represents the transition probabilities and hence the dynamics of S. Suppose also that S evolves into a complex superposition Ψ of its basis states, where in this example Ψ is (represented by) the normalized vector $1/\sqrt{5}(1, 2i)$. Then $\Psi+ = (1/5, 4/5)$. Multiplying the matrix M and Ψ+ together yields the following:

$$\begin{bmatrix} 1/2 & 1/3 \\ 1/2 & 2/3 \end{bmatrix}\begin{bmatrix} 1/5 \\ 4/5 \end{bmatrix} = \begin{bmatrix} 1/10 + 4/15 \\ 1/10 + 8/15 \end{bmatrix} = \begin{bmatrix} 11/30 \\ 19/30 \end{bmatrix}.$$

We argue that the Markov vector (11/30, 19/30) gives the correct probabilities 11/30 and 19/30 for the atomic transitions $\Psi\to A$ and $\Psi\to B$ respectively, using the following reasoning. We note first that $|\langle\Psi|u_1\rangle|^2 = 1/5$ and $|\langle\Psi|u_2\rangle|^2 = 4/5$, which is to say that the conditional probability of the atom being in state A, given that it is in state Ψ, is 1/5, and the probability that it is in B, given that it is in Ψ, is 4/5. $p(A|\Psi) = 1/5$ and $p(B|\Psi) = 4/5$. These probabilities are not transition probabilities, but reflect the A and B "aspects" of the superposition Ψ.

Secondly, there are two ways or "routes" by which an atom in Ψ can make the probabilistic transition to A. Either the "A-aspect" of Ψ makes the transition to A, or the "B-aspect" does. The probability for the atom to follow the first route is obtained by multiplying $p(A|\Psi)$ by the transition probability $p(A\rightarrow A)$, i.e. $1/5 \times 1/2 = 1/10$. The probability of the second route is $p(B|\Psi) \times p(B\rightarrow A) = 4/5 \times 1/3 = 4/15$. Since the two routes are mutually exclusive, we add 1/10 and 4/15 to get the total probability 11/30 of an atom in state Ψ jumping to A, i.e. for the transition $\Psi\rightarrow A$. Similar calculations yield 19/30 for $p(\Psi\rightarrow B)$. These are precisely the values assigned these transitions by the Markov vector (11/30, 19/30).

The calculation of these probabilities using Markov vectors and matrices opens up the possibility of an empirical test of the overall hypothesis of this paper, which is that atoms exhibit a discrete probabilistic evolution, not a continuous one. The test is this. Place a single trapped atom or ion in a known mathematical superposition Ψ of excited energy levels. Let A be the ground state, from which the electron is quickly driven into the fluorescent strong transition, and let B be the metastable "dark" state. Calculate the probabilities of the transitions $\Psi\rightarrow A$ and $\Psi\rightarrow B$ using the Markov methods of this section, and check in a series of trials whether the observed frequencies match the predicted probabilities.

(If it is more convenient to place the test atom in a mixed state D rather than a pure superposition, then the diagonal of the density matrix will serve equally well as the required Markov vector, from which the probabilities $p(D\rightarrow A)$ and $p(D\rightarrow B)$ can be obtained as before.)

9. Discrete atomic transitions: ontology or epistemology?

The present paper attempts to show that a consistent account can be given of energy changes in single atoms as Markov processes. In the course of the process the atom makes discrete transitions from one level to another in accordance with the probabilities of a Markov transition-matrix. Many investigators on the other hand, who are of the opinion that quantum mechanics precludes transitions of this kind having any ontological status, interpret the transitions as measurement-induced, or as characterizing our knowledge of the atom rather than the atom itself. See e.g. Javanainen (1986); Pegg, Loudon and Knight (1986); Cook (1990), pp. 401-407; Wiseman (1996), esp. pp. 205-208; Wiseman and Toombes (1999). A review and discussion of this approach is found in Home and Whitaker (1992), (1993).

Here are some quotes:

> "The atomic evolution described by the density-matrix elements is of course continuous, but the detection of the emitted photon immediately converts *a priori* probabilities into *a posteriori* probabilities, giving rise to discontinuities or jumps associated with the detection process." (Pegg, Loudon and Knight (1986), p. 4085)

> "It is tempting to go beyond the picture presented by the measured results and to ask questions such as, 'When did the quantum jump actually occur between the two measurements that gave different results?' But such questions are undoubtedly inappropriate because it is the measurement itself that projects the system into the new state. ... Hence, quantum jumps seem to be a property of the measurement process." (Cook (1990), p. 399)

The question of whether the sources of quantum jumps are instantaneous transitions in the atom, or alternatively the process of observation, comes to a head in the case of dark periods. If during a period of active fluorescence a dark period intervenes in which no photons are detected, do the probabilities P_1 and P_2 of being in levels 1 and 2 change? Not for dark periods of short duration, according to Cook (1990) p. 406, since it might be that the atom is in state $|1\rangle$ and simply has not yet emitted a photon. But as the dark period lengthens, there occurs a knowledge-induced probability shift, a "Bayesian transition", which gives the atom the new and longer expected lifetime of level 2 in place of the shorter lifetime of level 1.

These Bayesian changes in probability are in Cook's words "as 'real' as those caused by physical transitions". His claim is that, when an atom initially in any superposition of excited states is projected into the metastable state $|2\rangle$ by a Bayesian flow of probability, this constitutes "the quantum mechanical explanation of Dehmelt's intuitive shelving concept". Cook concludes (p. 407) that "It is interesting that the quantum formalism attributes electron shelving to the lack of fluorescence, whereas the intuitive picture of the process attributed the lack of fluorescence to electron shelving".

The majority view seems to be that discrete atomic transitions are not a feature of the physical world, but rather of our observation of the world. To this thesis there are a number of possible replies, among them the following.

(i) As is argued in this paper, it is possible to give a consistent account of the evolution of atomic systems as Markov processes. The appeal to photon detection as the source of discontinuous changes is therefore unnecessary.

(ii) Intuitively, one would think that atomic transitions in an atom cause photon emission, and photon emission causes a registration in a detector. Conversely, lack of an atomic transition (i.e. "shelving") causes lack of photon detection. To reverse these causal dependencies, and argue that electron shelving should be attributed to absence of photon observation, would be justified only if the intuitive idea that atoms undergo discontinuous transitions were subject to severe objections. However, the central thesis of this paper is that the discrete-transition model of atomic evolution is consistent, plausible and physical.

(iii) As is pointed out in Home and Whitaker, detection of photons emitted by an atom can take place at great distances away, and at times long after the apparatus used to contain the atom has been dismantled (1992, p. 2392; 1993, p. 115). One cannot "attribute quantum jumps to detection" if the system to which the transitions are attributed has ceased to exist before the detection takes place. In particular, it would be inconsistent to suggest that the atomic process itself is "driven by the act of observation" (1993, p. 115).

(iv) As is also noted in Home and Whitaker, those who claim that the behaviour of a physical system depends on the participation of an observer must be prepared to assert that the system would behave in a different fashion if unobserved (1992, p. 2392). But this seems implausible. How would one go about comparing the behaviour of an observed with an unobserved system? The standard procedure is to construct a theory of a system, e.g. a Markov model of atomic transitions, and then test the model by comparing predicted with observed effects, probability values, etc.

(v) Finally, one of the strongest arguments against the idea that atomic transitions are the product of measurement, and in favour of their ontological status, is the mathematical conclusion that Cook and Kimble come to in their (1985). This is, that in the V-configuration fluorescent system of section 1, both the "on/light" and "off/dark" times are distributed exponentially. This implies that a histogram plot should show an inverse exponential relation between length of period and number of periods of a given length. Furthermore, the difference in decay rates for the "on" and "off" states must be due to a process, such as spontaneous emission, which affects only the length of the *dark* periods (Erber et al. (1989), pp. 259-60). But if all this is so, then the evidence for identifying "dark period" with "atomic shelved state", as opposed merely to "absence of photon detection", becomes very strong. What reason, other than decay of an atomic energy state, could account for the precise exponential distribution of dark times?

10. Conclusion.

The objective of the paper has been to suggest explicit recognition of the presence of discontinuity in atomic evolution by giving an account of atomic transitions as Markov processes, and to deal with the objection that superpositions of energy states cannot be incorporated into processes of this kind. Amongst other things, this view implies that instantaneous transitions can be regarded as physical phenomena, and not simply as by-products of observational methods. The strongest argument for the "ontological" status of atomic transitions is the fact, noted in (v) of section 9 above, that the exponential distribution of dark periods in fluorescence is evidence that such periods are caused by exponentially decaying metastable states. In fact, both Nagourney, Sandberg and Dehmelt (1986), and Bergquist, Hulet, Itano and Wineland (1986) fit exponential curves to observed dark-time durations in order to obtain expected lifetime values of metastable states in barium and mercury ions. Without the identification of dark periods with the occupancy of "shelved" atomic states, the central reasoning on which these papers are based would be lost.

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