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Elementary processes in quantum mechanics, from a stochastic standpoint ([1])

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With 1 figure

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Abstract

The simplest Ansatz for the description of the creation and annihilation of a particle at a point leads to a stochastic equation that is equivalent to the corresponding quantum-mechanical equation. Since all equations of non-relativistic quantum mechanics are combinations of such elementary processes, quantum mechanics is implied by the definition of the elementary processes of “creation-annihilation” in the same way that NEWTONIAN mechanics follows from the definition of the elementary process of “infinitesimal motion.”

On 25-9-1911, ARNOLD SOMMERFELD proved to the assembled German naturalists and physicians, perhaps two years before BOHR’s fundamental work on the subject, that one should not connect energy with PLANCK’s constant, but the action integral, and in conclusion, stated: “However, I would not like to go so far as to see the true origin of *h* in this connection…Moreover, I would like to give preference to the opposite standpoint, that PLANCK’s *h* is not explained by molecular dimensions, but by the existence of molecules as functions and as a result of assuming an elementary quantum of action.”

This recollection of SOMMERFELD is welcome to me, since the title “elementary processes in quantum mechanics, from a stochastic standpoint” can arouse the suspicion that I would like to return to classical mechanics, so to speak. On the contrary, it shall be detailed how the stochastic character of quantum mechanics differs from that of classical statistical mechanics. Therefore, I shall restrict myself in the mathematical part to the examination of processes in the simplest physical systems, namely, the ones with only two properties such as spin, isospin, and the like, to which the alternative existence-nonexistence also belongs.

Due to their simplicity, such processes are treated repeatedly, especially in popular and philosophical papers. Here, they are recommended because they can be immediately compared to the alternatives that enter into in the theory of stochastic processes. I hardly

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([1]) From a colloquium talk in Karlsruhe, 22-2-1965.

need to explain what I mean by alternatives in stochastic theories. One thinks of the two sides of a coin, even and odd faces of a die, and the like.

The concepts of "stochastic" and "stochastic process" are still unfamiliar to physicists. In the Foreword to his book, the English mathematician J. L. DOOB said: "A stochastic process is the mathematical abstraction of an actual process whose evolution is governed by the laws of probability." Thus, in the future, we should no longer speak of "statistical mechanics," but of "stochastic mechanics," in physics. In fact, the word "statistics" is used by mathematicians only in connection with counting, but not with the concept of "probability."

I must confess my sin, that in the Festschrift on HEISENBERG's 60$^{\text{th}}$ birthday, I said that one could not associate the changes in probabilities in quantum mechanics with stochastic equations. At the time, I identified stochastic equations with MARKOV chains, master equations, PLANCK-KOLMOGOROV equations, or whatever else that they might be called. My assertion was correct for them. However, it was not true for arbitrary stochastic equations. In fact, the concept of "stochastic equations" is so far-reaching that it subsumes all equations for time-dependent probabilities, including the ones that will be developed here.

In the broader sense of the concept, the statement that the equations of quantum mechanics are stochastic is somewhat narrow in scope. It says only that we can derive how the probabilities change in time from the equations. As for the question of whether quantum mechanics can be derived from a classical one, all that is relevant is whether the von NEUMANN equation of quantum mechanics can be developed for a MARKOV chain. Nothing changes in our previous assertion, except that this is probably possible approximately, but not rigorously.

When we speak of elementary processes, we mean annihilation and creation processes, and thus processes in which a particle of a certain kind disappears or appears at a location in space. The state of a particle at a point will thus be described by two probabilities: Let $w_0(t)$, $w_1(t)$ be the probabilities for zero or one particles of the stated kind to exist at the point considered at time t, respectively. We would not like to speak of two particles at one point. If there were such a thing then we would briefly speak of two particles, three particles at a point, etc., of a new kind as a double particle, triple particle, etc., in order to not distinguish them. With that definition of particles, the Pauli Exclusion Principle will always be true, so we will have only two probabilities w_0 and w_1 for a particle type at a point, for which one will always have:

$$w_0(t) + w_1(t) = 1. \tag{1}$$

Thus, there is only one key number – say, the difference between the probabilities:

$$-1 \leq w(t) = w_0(t) - w_1(t) \leq 1, \tag{2}$$

which must always lie in the interval between – 1 and + 1. We ask: According to what law does $w(t)$ change in time? In this, we are assuming that it is, in principle, possible to determine $w(t)$ experimentally at every moment.

What properties must the equation have that links the probability differences at different times to each other? The linearity of the connection follows from the miscibility of statistical aggregates and from their virtual character. Since ignorance – i.e., $w = 0$ – cannot go to knowledge by merely waiting, $w = 0$ must be a stationary solution, and the equation for w must be homogeneous. It follows from the causality principle that $w(t)$ can depend upon only those $w(t')$ for which $t' \leq t$. We thus have:

$$w(t) = \int_{-\infty}^{t} K(t - t')\, w(t')\, dt', \tag{3}$$

if we consider the homogeneity of time, in addition.

This integral also subsumes differential equations, since one can allow K to be a distribution. The simplest differential equation has order one:

$$\dot{w}(t) = -\lambda\, w(t).$$

In this, the factor $-\lambda$ on the right-hand side must be less than 0, since otherwise $w(t)$ would increase exponentially, which would lead to a conflict with the inequality (2). Eq. (4) is the master equation for the alternative. It is certainly inconsistent with the quantum mechanics of elementary processes.

The integral kernel in eq. (3) has damped or undamped harmonic oscillations as its eigensolutions. From the inequality (2), no eigenvalue with a positive real part can occur; let negative real parts also be excluded. Indeed, decay processes are commonly characteristic in physics, and they are at the root of the entropy theorem, which is a collective phenomenon in statistical mechanics. Should that remain true, then the elementary process must contain no eigenvalues with negative real parts. In fact, this requirement has a deeply-rooted – I would like to say, philosophical – meaning. We shall first go into that in our the conclusion. Once again, here is the requirement: The eigenvalue must be purely imaginary or 0.

Since the integral kernel is real, it lies symmetrically about 0. Within the concept of "process" lies the fact that there must be at least one eigenvalue (so here, at least one pair $\pm i\Omega$) that is non-zero. We would like to interpret the concept of "elementary" by saying that there should be only one such pair. In that way, one will obviously get an oscillating function.

If one thinks of creation and annihilation processes for the motion of a particle in space, in particular, then the particle will be "here" at one moment and somewhere else before and after it. The location will then be empty for a long time, in such a way that there must be a solution w = constant $\neq 0$, along with the oscillating solution, and thus, a 0 eigenvalue, and indeed only one, in order to not forfeit the elementary character. Thus, the differential equation:

$$\dddot{w} + \Omega^2 \dot{w} = 0 \tag{4}$$

will enter in place of eq. (3). This equation, which is simple to understand, is equivalent to the von NEUMANN equation in the quantum mechanics of elementary processes.

We shall next show that the elements of the statistical matrix of quantum-mechanical elementary processes satisfy eq. (4) precisely. The von NEUMANN equation generally reads:

$$i\dot{P} = HP - PH. \tag{5}$$

P and H will be 2×2 matrices for an elementary process. They are Hermitian; P and H have traces 1 and 0, resp. We can then represent both of them in terms of PAULI matrices as follows:

$$P = \tfrac{1}{2}(1 + \mathfrak{p} \cdot \vec{\sigma}),$$
$$H = \tfrac{1}{2}\vec{\Omega} \cdot \vec{\sigma}. \tag{6}$$

It follows from this that:

$$H^2 = \tfrac{1}{4}\vec{\Omega}^2 = \Omega^2 \tag{7}$$

will be a real number. If we substitute that into the equation that emerges from eq. (5):

$$-\ddot{P} = H^2 P - 2\,H\,P\,H + P\,H^2$$

then the once-more-differentiated equation:

$$-\dddot{P} = H^2 \dot{P} - 2H\dot{P}H + \dot{P}H^2, \tag{8}$$

in connection with:

$$i\,H\,\dot{P}\,H = H^2\,P\,H - H\,P\,H^2 = P\,H^3 - H\,P\,H^2 = -(HP - PH)\,H^2 = -\dot{P}H^2,$$

will imply that all three summands on the right-hand side of eq. (8) will coincide. Together with (7), one will get:

$$\dddot{P} + \Omega^2 \dot{P} = 0, \qquad \Omega^2 = \vec{\Omega}^2, \tag{9}$$

in harmony with (4a).

Since the solutions of the von NEUMANN equation for a Hermitian 2×2 matrix with trace 1 include three givens, just like the stochastic equation for w, one can substitute the two equations for each other. If we substitute eq. (6) in (5) then it will follow that:

$$\dot{\mathfrak{p}} = \vec{\Omega} \times \mathfrak{p}. \tag{10}$$

If we identify p_3 with w:

$$w = p_3 \tag{11}$$

then it will follow from (10) that:

$$\dot{w} = \Omega_1\,p_2 - \Omega_2\,p_1, \tag{12}$$

and by differentiating this, and using (10):

$$\ddot{w} = \Omega_1\,(\Omega_3\,p_1 - \Omega_1\,p_3) - \Omega_2\,(\Omega_2\,p_3 - \Omega_3\,p_1),$$

so

$$\ddot{w} + (\Omega_1^2 + \Omega_2^2)\,w = \Omega_3\,(\Omega_1\,p_1 + \Omega_2\,p_2). \tag{13}$$

One finally obtains from (12) and (13) that:

$$p_1 = \frac{\Omega_1}{\Omega_3}\frac{\ddot{w} + (\Omega_1^2 + \Omega_2^2)\,w}{\Omega_1^2 + \Omega_2^2} - \frac{\Omega_2 \dot{w}}{\Omega_1^2 + \Omega_2^2}\,,$$
$$p_2 = \frac{\Omega_2}{\Omega_3}\frac{\ddot{w} + (\Omega_1^2 + \Omega_2^2)\,w}{\Omega_1^2 + \Omega_2^2} + \frac{\Omega_1 \dot{w}}{\Omega_1^2 + \Omega_2^2}\,. \qquad (14)$$

Thus, $\mathfrak{p}$ and P can be determined from $w(t)$ for a given $\vec{\Omega}$. Initially, only the magnitude of $\vec{\Omega}$ is fixed from eq. (9).

The vector $\mathfrak{p}$ then describes the instantaneous state of the statistical aggregate. Since $-1 \leq w \leq +1$, all conceivable states will lie in the slab between $p_3 = -1$ and $p_3 = +1$ (see Fig. 1). That state will then decompose into two classes that are characterized by the inequalities $|\,\mathfrak{p}\,| \leq 1$ ($|\,p\,| > 1$, resp.). They will be vectors inside (outside, resp.) the cross-hatched unit sphere.

Eq. (10) shows us that the changes of state in the space of the vectors $\mathfrak{p}$ are rotations around an axis with angular velocity Ω. For an adverse position of the rotational axis, the outside points can enter into the domain $|\,p_3\,| \leq 1$. That means that not all directions for the axis are admissible, such that the possible motions would depend upon the aggregate of state vectors. The virtual, merely imagined, aggregate would still have an effect upon physical phenomena here. That is not possible. Thus, the only admissible aggregates will be ones whose state vectors lie inside or on the unit sphere:

$$\mathfrak{p}^2 \leq 1. \qquad (15)$$

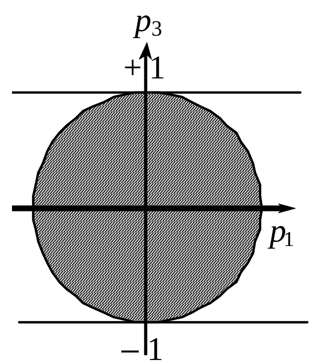

Fig. 1. The convex body of all aggregates.

This restriction has the consequence that one can derive not only the magnitude of the vector $\vec{\Omega}$, but also the angle ϑ with respect to the 3-axis, from observations. To that end, we consider the state in which the particle certainly does not exist at time $t = 0$, so $w(0) = +1$. Since that value cannot be exceeded, one must have:

$$w(t) = w(0) - \Omega^2\, t^2 + \ldots, \qquad (16)$$

for small times, so:

$$w(0) = 1, \qquad \dot{w}(0) = 0, \qquad \ddot{w}(0) = -\gamma\Omega^2 < 0. \qquad (17)$$

On the other hand, it follows from $w(0) = 1$, with the inequality (15), that:

$$p_1(0) = p_2(0) = 0, \qquad p_3(0) = 1, \qquad \mathfrak{p}^2 = 1. \qquad (18)$$

It then follows from eq. (14) that:

$$-\gamma\Omega^2 + \Omega_1^2 + \Omega_2^2 = 0, \tag{19}$$

i.e.:

$$\left| \mathfrak{e}_3 \times \frac{\vec{\Omega}}{\Omega} \right| = \sin\vartheta = \sqrt{\gamma}\,. \tag{20}$$

It emerges from eq. (19) that the azimuth of $\vec{\Omega}$ with respect to a plane the 3-axis will remain undetermined. It cannot be derived from $w(t)$, since the probability difference $w = p_2$ does not change under rotations around the 3-axis. For all experimentally-verifiable statements, all angles φ that we might substitute into:

$$\vec{\Omega} = (\sqrt{\gamma}\cos\varphi, \sqrt{\gamma}\sin\varphi, \sqrt{1-\gamma}) \tag{21}$$

will therefore be equivalent.

The vectors $\mathfrak{p}$ and $\vec{\Omega}$ are associated with the matrices P and H in a single-valued, invertible way. We have to ask: What follows from the inequality (15) for the matrix P? What consequences does the inequality of $\vec{\Omega}$ in eq. (21) imply for H?

As for the first question: It follows from eq. (6) that:

$$P^2 = P - \tfrac{1}{4}(1 - \mathfrak{p}^2), \tag{22}$$

so for an arbitrary one-column matrix Φ:

$$\Phi^+ P\,\Phi = \Phi^+ P^2\,\Phi + \tfrac{1}{4}(1 - \mathfrak{p}^2)\,\Phi^+\,\Phi \geq 0. \tag{23}$$

The von NEUMANN statistical matrix is then positive-definite. Thus, P satisfies not only the same equation as in quantum mechanics, but it also lies in the same domain of definition. The pure cases are defined by the outer surface of the domain $\mathfrak{p}^2 = 1$. Because it follows from eq. (22) that:

$$P^2 = P, \tag{24}$$

i.e., P is then idempotent, we can set:

$$P = \Phi\,\Phi^+, \qquad \Phi^+\,\Phi = 1. \tag{25}$$

In this, Φ is a one-column matrix, Φ^+ is its Hermitian conjugate, $\Phi^+\Phi$ is the Hermitian square of the vector Φ, and $\Phi\,\Phi^+$ is the dyadic product, which is a 2×2 matrix. One gets the SCHRÖDINGER equation for Φ:

$$i\dot{\Phi} = H\,\Phi \tag{26}$$

from the von NEUMANN equation in a known way. The probability difference is given by:

$$w = \Phi^+ \sigma_3 \Phi, \tag{27}$$

in this case, which is normalized by:

$$\Phi^+ \Phi = 1. \tag{28}$$

With $\Phi = \begin{pmatrix} \varphi_0 \\ \varphi_1 \end{pmatrix}$, $\Phi^+ = (\varphi_0^*, \varphi_1^*)$, it will follow from this that:

$$w_0 = \varphi_0^* \varphi_0, \qquad\qquad w_1 = \varphi_1^* \varphi_1. \tag{29}$$

Now, as for the second question: How does the indeterminacy of the azimuth of $\vec{\Omega}$ carry over to the SCHRÖDINGER operator H? We assert that it corresponds to the phase transformation:

$$H \to H' = D\,H\,D^+, \quad D = \begin{pmatrix} e^{i\alpha} & 0 \\ 0 & e^{i\beta} \end{pmatrix}, \qquad D^+ = \begin{pmatrix} e^{-i\alpha} & 0 \\ 0 & e^{-i\beta} \end{pmatrix}. \tag{30}$$

Starting from the equation that follows from (6):

$$\vec{\Omega} = \text{trace}\, H \vec{\sigma}, \tag{31}$$

we will obtain, by means of (30):

$$\vec{\Omega}' = \text{trace}\, H \vec{\sigma}', \qquad \vec{\sigma}' = D^+ \vec{\sigma}\, D \tag{32}$$

for the transformed vector, so:

$$\begin{aligned} \Omega_1' &= \quad \Omega_1 \cos(\alpha - \beta) + \Omega_2 \sin(\alpha - \beta), \\ \Omega_2' &= - \Omega_1 \cos(\alpha - \beta) + \Omega_2 \sin(\alpha - \beta), \\ \Omega_3' &= \quad \Omega_3 , \end{aligned} \tag{33}$$

so, by substitution of eq, (21):

$$\vec{\Omega}' = (\sqrt{\gamma}\cos(\varphi - \alpha + \beta), \sqrt{\gamma}\sin(\varphi - \alpha + \beta), \sqrt{1-\gamma}), \tag{34}$$

which is then just a change of the azimuth angle. The path from eq. (34) to (30) is also passable. The indeterminacy of the phase angle then corresponds immediately to the indeterminacy of the phase in the SCHRÖDINGER operator. A complete agreement between the stochastic description and the quantum-mechanical one also prevails in this.

With that, we have shown that a special third-order differential equation for the probability difference w of an alternative agrees with the quantum mechanics of so-called "dichotomic" systems, which are the systems with two possible states. For these simple systems, there is no doubt about the fact that we are dealing with objects that are sometimes in one state and sometimes in the other, and that in such simple cases, the probabilities do not satisfy wave equations, but oscillator equations. The object is the thing that is capable of changing the state, so the oscillator equation refers, not to the thing, but to the probabilities, which depend, not upon the state of the thing, but also upon our knowledge of it. It is only in that way that the statements of quantum mechanics are linked with the subject, and this, on the same basis as in any stochastic theory.

This thesis was first proved only for elementary processes. It will be true for all of quantum mechanics when one adds the postulate: All processes of quantum mechanics are combinations of elementary processes. In particular, one deals with annihilation and creation processes. A particle, possibly one of a different kind, vanishes or arises at each point of space. In the "classical" formulation, the alternative that all quantum mechanics is based upon then reads: "To be here or not to be here, that is the question."

If one accepts this postulate then that will yield the problem from which quantum mechanics can be derived, for many particles, as well as for ones that can arise and vanish. One achieves this with no special effort for non-relativistic theories. It should also be possible for relativistic theories. Up to now, that does not appear to be true, as if obstacles of a fundamental kind had been placed in the way. Thus, there are difficulties that originate in the fact that no satisfactory theory of relativistic particles exists yet. Here, one must await what the future might bring.

Our postulate, according to which, quantum-mechanical processes are combinations of creation and annihilation processes, shows that classical mechanics and quantum mechanics are already quite different in all relationships, and one can first fathom this when one returns to the beginnings of the philosophy of our cultural circle, and thus, about 2500 years ago. The basic question at the time was: "What constancy does the world confer upon all changes in events?" It can be answered in two contrary ways:

THALES of Milet (600 B. C.) and his followers considered everything that happened to be the motion of an unvarying substance. While some uncertainty prevailed in the nature of the substance, there was complete clarity about the event. The following law was then handed down by ANAXIMENES: "What changes – indeed, can something change at all – when it does not move?"

Perhaps 100 years later, HERACLITUS posed an opposite thesis, which was perceived by his contemporaries as indeed dubious, but which is most noteworthy for the physics of elementary particles. He rejected the concept of substance. Happening is not motion, but becoming and passing. The constancy of the world in not anchored in substance, but the law that governs all events. On that topic, he said with greater clarity: "One must build all that is common upon that, as a city is built upon its laws, and much more rigidly. All human laws draw their sustenance from a divine one that prevails to such an extent that everything obeys it, and it is stronger than everything." For some time, modern physics has been no stranger to the thought that the constancy of the world comes down to conservation laws.

Guided by experiment, in quantum mechanics, we have to choose, so to speak, the picture of phenomena that was conceived by HERACLITUS. It is likewise simple and clear how to get back to the classical mechanics of THALES. Both pictures belong to ideas that arise whenever one begins to grasp the world rationally. Naturally, we do not mean that venerability would be an argument for the one or the other picture, but probably that both of them reflect basic structures of thought in which one can remain, and not need to go back and forth between.

What we know about quantum mechanics today can be derived from the picture in which phenomena are a result of a succession of creation and annihilation processes. Since one then arrives at a self-contained theory in that way, there is no apparent basis for wanting to go back from the elementary creation and annihilation processes in the sense of THALES to motions, and no criterion that could save us from mere speculation, but probably experiments, which are completely incompatible with the THALES conception of things. One thinks of processes such as:

$$\pi^{-} + p \rightarrow \pi^{-} + p + \pi^{0},$$

in which nothing happens as a result of the process except that a new particle is added to the ones that are present.

All the same, SCHRÖDINGER had a charming idea about how one can understand the creation and annihilation of particles as processes of motion, namely, that particles can be compared to foam crowns on the water. Who knows? Perhaps, we must master the physics of water in order to be done with the problem of relativistic foam crowns. However, one must first know whether the quantum mechanics of relativistic particles is not actually ascertainable with the help of elementary processes. Although there are still-unsolved problems in it, there is much that suggests that such is not the case. We expect that the theory of relativistic particles can still be formulated with the means that have been worked out in quantum mechanics.

"Undoubtedly," we can, almost as in SOMMERFELD's Karlsruhe lecture, conclude that "our theoretical intuitions" about the quantum theory of relativistic particles "are found in a somewhat vague, transitional stage. However, scientific optimism, which is the basic principle for any advance, obliges us to believe that the vagueness will abate in the not-so-distant future, and the basic physical principles will then lie before our eyes in a much brighter light!"

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