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STOCHASTIC PROCESSES AND QUANTUM MECHANICS

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In this paper we shall briefly review various aspects of the interaction between the theory of stochastic processes and Quantum Mechanics. In order to get a clear picture it is very important to distinguish from the start two situations :

a) Stochastic processes as a description of the real world alternative to the usual interpretation of quantum mechanics (even though mathematically equivalent).

b) Stochastic processes as a mathematical tool useful for representing quantities of interest to quantum mechanics.

In the following we consider the two aspects separately and only in the end we comment on the relationship between them. Most of the material discussed here was developed in collaborations with G.F. De Angelis, F. Martinelli, E. Scoppola and M. Sirugue.

I - STOCHASTIC PROCESSES AS A REPRESENTATION OF THE REAL WORLD.

1. Stochastic Mechanics of a Scalar Particle.

Standard Quantum Mechanics is a probabilistic theory of the microscopic world in the sense that its connection with experiments relies on a frequency interpretation of the wave function. It is not however a probabilistic theory in its mathematical structure which is not immediately reducible to a theory of stochastic processes in a given probability space. This situation has stimulated over the years numerous attempts to introduce ordinary probabilistic concepts and constructions that could account for the previsions of Quantum Mechanics. A particularly successful one was the formulation on the part of Nelson [12] of a theory based on diffusion processes which is mathematically equivalent to the Schrödinger description of a scalar particle, i.e. of a particle without internal degrees of freedom. We start by giving an unconventional presentation of Nelson's basic idea.

Consider the Schrödinger equation for a charged scalar particle in an electromagnetic field

$$i\hbar\partial_t\psi = \frac{1}{2m}(-i\hbar\nabla - \frac{e}{c}A)^2\psi + V\psi \qquad (1)$$

A basic consequence of (1) is the continuity equation for the probability density $|\psi|^2$

$$\partial_t|\psi|^2 = -\nabla[\frac{\hbar}{m}\mathrm{Im}(\bar{\psi}(\nabla - \frac{ie}{\hbar c}A)\psi)] \qquad (2)$$

and this will be the starting point of our construction. Suppose we want to interpret $|\psi(x,t)|^2 = \rho((x,t)$ as the probablity density at time t associated to a Markov process described by a transition function $P(x',x,t)$ in such a way that

$$\rho(x,t) = \int\rho_o(x')\, P(x',x,t)dx' \qquad (3)$$

where $\rho_o(x)$ is some initial distribution. Then ρ must satisfy a Fokker-Planck equation

$$\partial_t\rho = \frac{\nu}{2}\Delta\rho - \nabla(b\rho) \qquad (4)$$

where ν is the diffusion coefficient and b a velocity field (drift). Comparing (4) and (2) we see that such an identification is possible if we take $\nu = \hbar/m$ and b satisfying

$$\nabla[|\psi|^2(b - \frac{\hbar}{m}\frac{\mathrm{Im}(\overline{\psi}(\nabla - \frac{ie}{\hbar c}A)\psi)}{|\psi|^2})] = \frac{\hbar}{2m}\Delta|\psi|^2 . \tag{5}$$

The solution of (5) is not unique. However if we require that b is a gradient when $A = 0$ we obtain the unique answer

$$\begin{aligned} b &= \frac{\hbar}{m}\nabla \ \ell n \ |\psi| + \frac{\hbar}{m}\frac{\mathrm{Im}(\overline{\psi}(\nabla - \frac{ie}{\hbar c}A)\psi)}{|\psi|^2} \\ &= u + v . \end{aligned} \tag{6}$$

Since u and v are given explicitely in terms of the wave function ψ, from the Schrödinger equation we obtain their equations of motion

$$\begin{aligned} \partial_t u &= -\frac{\hbar}{2m}\nabla(\nabla v) - \nabla(u.v) \\ \partial_t v &= -\frac{1}{m}\nabla V + \frac{1}{2}\nabla(u^2 - v^2) + \frac{\hbar}{2m}\Delta u \end{aligned} \tag{7}$$

The stochastic process associated to b via (4) can be described also in terms of the stochastic differential equation [12]

$$dx = b dt + \sqrt{\frac{\hbar}{m}}\, dw \tag{8}$$

where dw is the Wiener process.

At this point (7) and (8) (or (4)) constitute a self-contained scheme which can be used as an alternative to the usual quantum mechanical formalism. We shall comment later on the computational effectiveness of the new scheme. The fundamental question facing the physicist is whether the stochastic processes we have constructed have any "reality" which could imply eventually a new interpretation of microphysics. An answer to this question is not simple. A first step should consist in my opinion in a systematic reinterpretation of basic quantum mechanical observables in terms of concepts which are natural from the standpoint of diffusion processes. Already at this stage there are various aspects to consider. For example the energies of the excited states can be related, as Nelson did originally, to certain non ergodic processes corresponding to their wave functions. On the other hand they also describe the relaxation times of the process associated to the ground state*. They can be related therefore to exit times of the ground state process from space domains bounded by the nodal surfaces of the higher wave functions [9]. In other words one may take the attitude that measuring energy levels means measuring indirectly certain features of the ground state process. However the process itself does not seem to be directly accessible to observation if one translates the usual rules for the interpretation of quantum mechanics into the stochastic language. We cannot in fact measure the correlation between the values of the process at different times t_1 and t_2 because any attempt to localize the particle changes the velocity field b. Therefore after the measurement at t_1 we have a different process.

All this does not exclude the possibility that pushing the stochastic language to its natural consequences one arrives at new questions or generalizations, meaningless or unnatural for the standard interpretation of quantum mechanics, but susceptible of experimental test.

2. Stochastic Mechanics of a Spin 1/2 Particle.

For some time it was thought that it would be difficult to extend stochastic mechanics to particles with internal degrees of freedom e.g. to spin 1/2 particles obeying the Pauli equation(+)

$$i\partial_t \psi = \frac{1}{2}(-i\nabla - A)^2\psi + V\psi - \frac{1}{2}\underline{H}.\underline{\sigma}\psi \tag{9}$$

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \psi = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}$$

The reason for this belief was the lack of a classical analog for the spin. It turned out however that using the strategy previously indicated for the scalar case, the problem can be solved in a straightforward way simply by introducing discrete processes to describe the

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* This holds when $A = 0$

(+) To simplify the subsequent discussion we set all the physical constants equal to 1 .

internal degrees of freedom.[5].

Consider for simplicity the case $\underline{H} = \underline{const}$.
Then we can write $\psi(x,t,\sigma) = \varphi(x,t)\chi(\sigma,t)$, $\sigma = \pm 1$ where φ satisfies the Schrödinger equation (1) and χ

$$i\frac{d\chi(\sigma)}{dt} = -\frac{1}{2}[H_z\ \sigma\chi(\sigma) + (H_x - i\sigma H_y)\chi(-\sigma)] \tag{10}$$

There is a continuity equation associated to (10)

$$\frac{d|\chi(\sigma)|^2}{dt} = \mathrm{Im}[(H_x + i\sigma H_y)\chi(\sigma)\overline{\chi}(-\sigma)] \tag{11}$$

The idea is the same as before : we try to interpret (11) as a discrete Fokker-Planck equation (Kolmogorov forward equation) for $\rho(\sigma) = |\chi(\sigma)|^2$

$$\frac{d\rho(\sigma)}{dt} = -p(\sigma,t)\rho(\sigma) + p(-\sigma,t)\rho(-\sigma) \tag{12}$$

where $p(\sigma,t)$ is a transition probability per unit time. The comparison of (12) and (11) gives the essentially unique choice for p

$$p(\sigma,t) = \frac{1}{2}\{[H_x^2 + H_y^2]^{\frac{1}{2}} \left|\frac{\chi(-\sigma)}{\chi(\sigma)}\right| + \mathrm{Im}(H_x - i\sigma H_y)\frac{\chi(-\sigma)}{\chi(\sigma)}\} \tag{13}$$

One can then easily find the analogues of u and v

$$\begin{aligned} r &= H_z + \sigma\,\mathrm{Re}((H_x - i\sigma H_y)\chi(-\sigma)/\chi(\sigma)) \\ s &= -\sigma\ \mathrm{Im}((H_x - i\sigma H_y)\chi(-\sigma)/\chi(\sigma)) \end{aligned} \tag{14}$$

which obey the equations of motion

$$\begin{aligned} \frac{dr}{dt} &= -\ \sigma r s \\ \frac{ds}{dt} &= -\frac{1}{2}\sigma|H|^2 + \frac{1}{2}\sigma(r^2 - s^2) \end{aligned} \tag{15}$$

Notice the similarity in structure with (7) if one interprets ∇ as multiplication by σ . In terms of r and s the transition probability reads

$$p(\sigma,t) = \frac{1}{2}[(s^2 + (r - H_z)^2)^{\frac{1}{2}} - \sigma s] \tag{16}$$

Not all the solutions of (15) have the structure (14) so that an additional condition has to be imposed. For this point we refer the reader to [5].

A characteristic feature in the above construction is the appearance of the ratio $\chi(-\sigma)/\chi(\sigma)$. According to Cartan [3] there is a geometric meaning associated to it. Introduce the so called isotropic vectors associated to spinors

$$\begin{aligned} Z_1 &= \chi(\sigma)^2 - \chi(-\sigma)^2 \\ Z_2 &= i(\chi(\sigma)^2 + \chi(-\sigma)^2) \\ Z_3 &= -2\chi(\sigma)\chi(-\sigma) \end{aligned} \tag{17}$$

which satisfy the equation

$$Z_1^2 + Z_2^2 + Z_3^2 = 0 \tag{18}$$

This is a cone and the ratio $\chi(-\sigma)/\chi(\sigma)$ defines a generator of the cone. If we introduce now the complex variable $Z = r + is$ equation (15) takes the very simple form

$$i\frac{dZ}{dt} = \frac{1}{2}\sigma|H|^2 - \frac{1}{2}\sigma Z^2 \tag{19}$$

which can be interpreted geometrically as an equation of motion for a generator of the isotropic cone.

The general case of an inhomogeneous magnetic field can be treated along similar lines. The picture which emerges is that a spin $\frac{1}{2}$ particle can be described stochastically as a Brownian particle with two internal states moving in a velocity field which depends on the internal state. The latter changes at random times which in turn depend on the motion of the particle. The equations for the general case can be found in [5].

3. Calculations with Stochastic Mechanics.

Although of great conceptual interest, the above scheme could not pretend to be a real alternative to quantum mechanics if it did not provide effective calculational tools. Actually an approach based on (7) and (8) has been crucial in the study of certain aspects of the semiclassical limit of quantum mechanics i.e. the limit $\hbar/m \to 0$ [9,10]. Apparently there are two main reasons for that. The singular perturbation problem associated with (7) for $\hbar/m \to 0$ is less difficult than the corresponding one for the Schrödinger equation, in spite of the non linearity of (7). The stochastic equation (8) in the limit $\hbar/m \to 0$ can be studied with the powerful techniques of small random perturbations of dynamical systems. In this way new features of the semiclassical limit were discovered like tunneling instability due to localized deformations of the potential. Quite generally an approach based on (7) and (8) seems to be very effective for a qualitative understanding of the semiclassical limit. In fact there are several concepts from the theory of stochastic processes which provide a natural and intuitive basis for a description of the mechanisms involved. It may be an effective approach also to the study of disordered quantum mechanical systems[11].

II. STOCHASTIC PROCESSES AS AUXILIARY REPRESENTATIONS :

The Feynman-Kac Formula and its Descendants.

As long as we are interested in spectral properties the imaginary time Schrödinger equation (heat equation) is and has been a very powerful source of information. The reason, as it is well known, is the probabilistic interpretation associated to a large class of parabolic equations. A central role in this approach has been played by the so-called Feynman-Kac formula which gives the prototype of probabilistic expressions for the solutions of these equations.

For the imaginary time Schrödinger equation

$$\frac{\partial\psi}{\partial t} = (\tfrac{1}{2}\Delta - V)\psi = -H\psi \qquad (1)$$

the Feynman-Kac formula reads

$$\psi(x,t) = E\left(e^{-\int_o^t V(x+W_s)ds}\,\psi_o(x+W_t)\right) \qquad (2)$$

where ψ_o is the initial condition and the expectation is taken with respect to the Brownian motion of variance 1 starting at 0 for $t = 0$. To verify that (2) is the solution of (1) one proves that it defines a semigroup and then uses Ito calculus. There have been important applications of (2) in the qualitative study of the spectrum and eigen-functions of H[13]. An obvious question then is whether a generalization of (2) is possible for the imaginary time Pauli equation

$$\partial_t\psi = -\tfrac{1}{2}(-i\nabla - A)^2\psi - V\psi + \tfrac{1}{2}\,\underline{H}\cdot\underline{\sigma}\psi \qquad (3)$$

The previous experience with the stochastic mechanics of spin suggests that besides the expectation with respect to the Brownian motion, the formula for the solution should contain an expectation with respect to a standard jump process (Poisson process) for a selected component of the spin. This idea turns out to be correct and the solution of (3) can be written [6]

$$\psi(x,\sigma,t) = e^{\lambda t}\,E\{e^{-\int_o^t V(x+W_s)ds - i\int_o^t A(x+W_s)dW_s}$$

$$\cdot\, e^{\frac{1}{2}\int_o^t H_z(x+W_s)(-1)^{N_s}\sigma ds + \int_o^t \log[\frac{1}{2\lambda}(H_x(x+W_s) - i\sigma(-1)^{N_s}H_y(x+W_s))]dN_s}$$

$$\cdot\,\psi_o(x+W_t, \sigma(-1)^{N_t})\} \qquad (4)$$

where N_t is the standard Poisson process of parameter λ. In the following we shall take $\lambda = 1$(+).

(+) In concrete cases the arbitrariness of λ can be used to introduce a time scale natural for the problem.

Generalizations can be written down easily for equations where the wave function has more then two components[6]. A representation like (4) is interesting because the algebra connected with the Pauli matrices has been replaced by the expectation with respect to the Poisson process and no chronological product is necessary.

We now try to convey the flavour of what can be done with expressions like (2) and (4) by considering a simple application and some prospective generalizations of physical interest.

There is a very simple inequality which follows from (4) by taking the absolute value

$$|\psi(x,\sigma,t)| \leqslant e^{t} E\{ e^{-\int_o^t V ds + \frac{1}{2}\int_o^t H_z (-1)^{N_s} \sigma ds} \cdot e^{\int_o^t \log\, [\frac{1}{2}(H_x^2 + H_y^2)^{\frac{1}{2}}] dN_s} \; |\psi_o(x + W_t, \sigma(-1)^{N_t})| \tag{5}$$

which implies the following inequality for the lowest eigenvalue of the Pauli Hamiltonian

$$E_o(A,\underline{H}) \geqslant E_o(0,\underline{H}') \tag{6}$$

where $\underline{H}' = (\sqrt{H_x^2 + H_y^2}\,,\, 0\,,\, H_z)$.

In words it compares the behaviour of a charged spinning particle in an arbitrary electromagnetic field with that of a neutral particle in a planar magnetic field.

To illustrate the possible uses of inequalities like (5) and (6) let us make a rough estimate by taking in (5) the max with respect to σ and performing explicitely (now it is possible) the Poisson integration. We obtain

$$|\psi(x,\sigma,t)| \leqslant E\{e^{-\int_0^t V ds + \frac{1}{2}\int_0^t |H_z| ds} \cdot e^{\frac{1}{2}\int_0^t (H_x^2 + H_y^2)^{\frac{1}{2}} ds} \operatorname*{Max}_{\sigma} |\psi_o(x + W_t, \sigma|\} \tag{7}$$

$$= E\{e^{-\int_0^t \overline{V} ds} \operatorname*{Max}_{\sigma} |\psi_o|\}$$

where the expectation is taken with respect to the Brownian motion only with an obvious definition of $\overline{V}$. Our original semigroup is now majorized by the evolution of a scalar Schrödinger equation with an effective potential $\overline{V}$. It is well known[2,13] that if

$$\operatorname*{Sup}_{x} E\{\int_0^\infty |\overline{V}_-(x + W_s)| ds\} < 1 \tag{8}$$

where $\overline{V}_-$ is the negative part of $\overline{V}$, the spectrum of the Hamiltonian associated with $\overline{V}$ does not include eigenvalues $\leqslant 0$. But this in turn implies that also our original problem does not have such eigenvalues due to the inequality for ground states, analogous to (6), $E_o(A,\underline{H}) \geqslant E_o(\overline{V})$ implied by (7). It is clear in this connection that it would be important to exploit in a more effective way the explicit representation of the spin dynamics provided by (4) to obtain conditions on the absence of negative spectrum less stringent then (8).

Here is a situation where this type of information would find interesting applications.

Let M be a Riemaniann manifold of dimension n, $\wedge^p$ the associated space of p-forms, $p = 0,1, \ldots, n$, d and d^* the operation of exterior derivative and its adjoint. Then, as shown by Witten [14],

$$Q_1 = d + d^*$$

$$Q_2 = i(d - d^*)$$

$$H = dd^* + d^*d$$

$$Q_1^2 = Q_2^2 = H$$

$$Q_1Q_2 + Q_2Q_1 = 0$$

constitute what physicists call a supersymmetric structure. The zero eigenvalue equation $H\omega = 0$ for harmonic p-forms can be written in local coordinates[15]

$$g^{jk}\,(D_j, D_k, \omega)_{i,\ldots i_p} - \Sigma_{s=1}^{p}\ \omega_{i,\ldots i_{s-1}\, j\, i_{s+1}\ldots\, i_p} R^{j}_{i_s} \tag{10}$$

$$- \Sigma^{p}_{s<t=1}\ \omega_{i,\ \ldots\ i_{s-1} j\ i_{s+1}\ \ldots\ i_{t-1}\ k i_{t+1}\ \ldots\ i_p} R^{jk}_{i_s i_t} = 0$$

where R is the curvature tensor.

Its time dependent version has therefore the form of Pauli type equations considered in[6]. Physicists are interested in knowing whether such forms exist in L_2 for any p. If they do not exist they say that the supersymmetry is dynamically broken. From the geometrical point of view this corresponds to the vanishing of cohomology groups. In view of the previous discussion the generalized Feynman-Kac formulae may be an interesting tool for the study of such problems continuing the work initiated by Malliavin, Berthier, Gaveau, Vauthier[16] .

III. CONCLUSIONS.

First of all one should emphasize that the topics discussed do not exhaust all the connections between stochastic processes and quantum mechanics. The aspects considered reflect taste and personal experience of the author. Among the topics which have been left out I should mention the very important connection between the Feynman integral and Poisson processes first pointed out by Maslov then reformulated and considerably extended in recent years by the Marseille group[4]. This approach based on Poisson processes with jump amplitudes varying in a continuous way preserves in some sense the structure of the classical phase space and may be important for the study of quantum evolutions close to classical trajectories when $\hbar \to 0$.

In this paper we have sharply distinguished between the uses of stochastic processes as a representation of reality and as auxiliarly tools. Then one may ask whether there is any relationship between these different aspects. Some years ago Guerra and Ruggiero[7] made the intriguing remark that in certain simple cases the stochastic process associated to the imaginary time Schrödinger equation is essentially the same as the process associated to the ground state by stochastic mechanics (they are described by unitarily equivalent semigroups). This seemed to open the way to a "realistic" interpretation of Euclidean theory. The situation now is that for the case of scalar Schrödinger particles the connection is generally true and well studied mathematically[1].
It seems to fail however for a scalar particle in an electromagnetic field and for a Pauli particle in an arbitrary magnetic field. In my opinion this question requires further clarification.

In concluding we would like to mention an important problem connected with stochastic mechanics. To what extent can be given a natural mathematical formulation without invoking quantum mechanics ? Various people over the years have noticed that an answer to this question might exploit certain similarities with problems in stochastic control theory. A rather complete formulation of this aspect for the case of scalar particles has been given finally by Guerra and Morato[8] .

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