

## On decoherence theory

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This note supplements the lecture delivered at Academia das Ciências de Lisboa, November 27, 2009, on the interpretation of quantum mechanics. Although decoherence has been briefly referred to in the lecture, it has not been included in the resulting chapter "*The Interpretation of Quantum Mechanics Revisited*", in "*Quantal Aspects of Chemistry and Physics*", Chapter 5, pgs. 45-77 (eds. J.Redinha; J. da Providência; A.Varandas), *Coimbra University Press*, 2011.

Classical mechanics states that the positions ( $q_i$ ) and momenta ( $p_i$ ) of a N-particle system ( $i = 1, 2, \dots, N$ ) are precisely defined simultaneously at any instant. So are other dynamical properties, functions of positions and momenta. The state of the system at time  $t$  is defined by the set of values  $[q_i(t), p_i(t)]$ , i.e., it is identified with observable variables.

An experimental measurement on the system reveals the values of the properties that otherwise would remain unknown, though well-defined. The measuring device just "look" and register what the values really are. Any measurement has, of course, ever-present uncertainties but the real values of the properties can always be estimated by treating the random errors.

Ultimately, we do not even need to make *successive* experimental measurements. It suffices to know precisely the initial positions and momenta of the particles (for instance, by a measurement at the starting instant) and to resolve the motion equations from there on. Then, we should be pretty certain about the values of the properties of the system at any posterior instant. So, a measurement would be no more than a confirmation of what we already know. Alternatively, Liouville's equation can project the system in phase space and work out the respective probability density functions.

Whatever the choice, one point seems clear: in the classical picture a measurement device is just *one of the tools* to know the properties of the system assuming that their real and ever-deterministic values are not significantly affected.

Is this strictly acceptable? Indeed, a measurement device interacts, so the observed system certainly loses its eventual isolation. In principle, one should somehow include additional terms into the motion equations for describing the interactions, predict and explain the observations: why "this" and not "that" value? No such need for classical mechanics: the device disturbances can always be reduced to a minimum and the values of the properties are already "imprinted" upon the particles at any instant. Thus, just "look and register" with no further worry.

Classical statistical mechanics do not neglect, however, the role of the environment in non-isolated systems. It is introduced explicitly into the probability density functions or in the molecular dynamics equations of motion, considering different constraints (e.g. temperature, pressure and chemical potential). Average values and molecular trajectories are then predicted for comparison with experimental observations. Nevertheless, the *explicit* consideration of the measuring devices is generally absent, supposedly accounted for the estimation of random errors. The observer/device appears like an outsider to the system that flows independently "out-there". In other words, it is assumed that the information about a given system can be obtained without influencing its state.

The structure of the orthodox (conventional) quantum mechanics is quite different. The state of a system is not identified by a set of observable variables (as in classical mechanics) but by a vector  $|\Psi(q_i; t)\rangle$  of Hilbert's space, where the  $q_i$ 's are "dummy" position variables. The physical properties are represented by linear Hermitian operators, and the positions and momenta, for example, are no longer well-defined, simultaneously and precisely, at a given instant. The only possible observable values ( $A_k$ ) for a property  $A$ , represented by operator  $\hat{A}$ , are the solutions of the eigenvalue equation:

$$\hat{A} |\alpha_k\rangle = A_k |\alpha_k\rangle \quad (k = 1, 2, \dots)$$

where the  $|\alpha_k\rangle$ 's are the eigenvectors constituting a *basis* of Hilbert's space. As such, an arbitrary *pure* state  $|\Psi\rangle$  can be represented by a *coherent superposition* of these *pure* basis vectors:

$$|\Psi\rangle = \sum_k |\alpha_k\rangle \langle \alpha_k | \Psi \rangle$$

Now, two postulates of quantum mechanics:

- a) If  $A$  is measured on an arbitrary state  $|\Psi\rangle$ , the strongest predictive statement that can be made is that the probability of obtaining the value  $A_k$  is  $|\langle \alpha_k | \Psi \rangle|^2$ .
- b) A measurement generally changes *non-deterministically* the state vector. Regardless of the state before the measurement, *immediately* after it the new state will coincide with the eigenvector corresponding to the obtained eigenvalue (this is the so-called *reduction* or *collapse* of the state vector).

The postulates mean that the direct link between cause and effect is broken. This is the big clash with classical mechanics. In fact, it is implied that measurements on *exactly* the same state may give different results. Only if the state vector coincides with an eigenvector of the operator  $\hat{A}$ , for example  $|\alpha_i\rangle$ , can one be certain that *repeated* measurements of the observable  $A$  give always the same result,  $A_i$ . However, in that state, repeated measurements of another observable  $B$ , whose operator,  $\hat{B}$ , does not commute with  $\hat{A}$ , may give different results for  $B$ .

Quantum mechanics, contrary to classical mechanics, assumes the role of the measuring device, though only *postulating* its effect. Nothing in the *original* mathematical structure of the theory explains how and when the state vector collapses leading to the selection of the observed eigenvalue. This is very uncomfortable and raises puzzling questions.

The measuring device should be an inseparable part of the observed system, constituting with it an isolated super-system. If one follows the time evolution of the pure state vector of such an isolated super-system, by Schrödinger's equation (or the equivalent time-evolution operator), a succession of entangled states is obtained, and the *non-unitary evolution (collapse)* of the total state vector, assumed by postulate b), does not turn out. This seems expectable since the time-evolution operator is *unitary*, i.e., it preserves the relationships of the phase angles (*coherence*) of the initial state vector. However, it is a striking issue mainly for cosmologists leading to many quantum formulations, from the relative-states (many-worlds) to the actual M-theories.

Let's turn to quantum statistical mechanics. Consider an *ensemble* of very many systems each in the same pure state  $|\Psi\rangle = \sum_k |\alpha_k\rangle \langle \alpha_k | \Psi \rangle$ . The ensemble is also described, initially, by a pure *ensemble-state* vector which, according to the unitary time-evolution, would always remain pure. After a measurement of property  $A$ , in every member of the ensemble, each system shall *experimentally* be found in one of the possible pure eigenstates  $|\alpha_k\rangle$  with probability  $|\langle \alpha_k | \Psi \rangle|^2$ . Yet, as the measurement is non-unitary the initial relationship of the phase angles of the pure state is not preserved. Therefore, for most of the situations, the ensemble is projected into a *statistical mixture of (incoherent) pure states* precluding, particularly at macroscopic scales, the occurrence of interference (Schrödinger's cats). The statistical mixture is no longer described by a pure ensemble-state vector, otherwise such "cats" would frequently be observed.

Either a statistical mixture of states or a pure state can be described by *density matrices* ( $\rho$ ), the

fundamental tools of decoherence theory. Put simply, in a coherent superposition of pure states, the off-diagonal elements of the density matrix (meaning interferences) are non-zero, whereas for a statistical mixture of incoherent pure states they are zero (expressing what is observed under most practical laboratory conditions).

Essentially, decoherence theory aims to reach the *classical-like* limit of quantum dynamics through a continuous reduction (*decoherence*) from the coherent density matrix to the incoherent density matrix that describes the statistical mixture of states observed in the laboratory. To this end, the influence of the outside world (environment plus observer) on the system can be formalized by adding relaxation terms to von Neumann's equation:

$$\frac{d\rho}{dt} = \frac{1}{i\hbar} [H_{\text{int}}, \rho] + \text{relaxation terms}$$

(the relaxation terms are added phenomenologically to account for the ensemble aspects of the problem)

Then, it is expected that the preferred basis of the measurements (the *pointer basis*) is *robustly* singled out and that decoherence prevents the coherent superposition of the basis vectors from persisting.

It is noteworthy that this formulation does not seem to change the fundamental structure of the conventional quantum mechanics. It resembles what is done in classical statistical mechanics by introducing additional terms to Newton's, Hamilton's, Lagrange's or generalized Liouville's equations, in order to account for different environments, not appearing to alter the fundamental structure of classical mechanics.

In the context of decoherence theory striking conclusions are drawn. For example, the so-called collapse of the state vector appears not as an instantaneous projection to a particular measurement eigenstate but rather as a physical process taking a finite time. Thus, decoherence times can be estimated indicating how fast or slow decoherence processes might take depending on the type of environment and interactions. For most macroscopic systems the decoherence process is generally so fast that can be assumed instantaneous. In contrast, at mesoscopic scales there are systems that may even be caught in the process of coherence decaying. Moreover, other systems may only decohere in huge times.

The picture coming from decoherence theory alleviates, at least to me, the spiritual discomfort of postulate b). Of course, one can adopt an instrumentalist-pragmatist-positivist standpoint and apply the postulate straight away. After all, in practical terms, is what the majority of people do: as the recipe works very well let's use it as it is. Nevertheless, I believe that human mind requires more, and some of this "more" seems to be offered by decoherence theory. Incidentally, should not postulate b) be rephrased by dropping the words "non-deterministically" and "immediately"?

There are, of course, criticisms on decoherence theory. Here, we do not delve into them but outline one related to that postulate:

"Decoherence theory eliminates interferences but, even so, all possible results  $A_i$  are left valid:  $A_1$  and  $A_2$ ...and  $A_k$ ...and...The orthodox formulation, on the contrary, asserts that the choice is undetermined before the measurement (all outcomes are valid:  $A_1$  and  $A_2$ ...and  $A_k$ ...and...) however determined after the measurement, i.e., *only one* outcome is observed ( $A_1$  or  $A_2$ ...or  $A_k$ ...or...). Decoherence theory does not provide a mechanism explaining how "and" becomes "or", therefore does not solve properly the measurement problem".

The orthodox interpretation states that after the measurement "and" becomes "or" but *without explaining* "how" this happens, only postulates the fact frequently observed at least in most

laboratory conditions. Moreover, it is suggested that the process is instantaneous and at random.

This is not so for decoherence theory. The reason of the elimination of interferences is explained (by means of the ever-lasting interactions within system  $\cup$  external world), illustrating *how* and *why* the *classical-like* limit of quantum dynamics can turn out; it also suggests that the physical process is not totally at random. Furthermore, it is able to work out decoherence times, showing that the process is not instantaneous. Yet, like the orthodox interpretation, it neither gives a mechanism explaining *why* only one outcome is observed nor predicts its value.

The last point, however, seems *unanswerable* by decoherence theory. In fact, its formulation is within the mathematical structure of the conventional quantum mechanics. Thus, the probabilities of the reduced density matrix, though similar to the classical ones, remain quantum probabilities, i.e., they are just *classical-like* probabilities. As such, they do not express a *lack of knowledge* of the precise initial state, and of other details, that once known would predict (like in classical mechanics) the single outcome of a measurement.

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