Measurement, Density Matrix and Decoherence

Schrödingers cat in quantum mechanics is an illustration for the property of quantum mechanical objects that they may be in undecided states, represented by the cat being simultaneously dead and alive. These are called examples of coherence or quantum interference.

When an object is much bigger than a quantum particle, however, we encounter it as a classical object, the cat is either dead or alive, being in each of these two states with some probability. The question now arises, how this difference between a quantum object and a classical object arises. Alternatively we may ask, how the undecided quantum state changes into a decided (incoherent) state, when the quantum object interacts with the (large) measurement apparatus, a classical environment.

The expectation value $< A >$ of an observable (or equivalently an operator) A, when the system is in a state defined by the wavefunction $|\psi >$, is written as

$$< A >=< \psi|A|\psi > \tag{1}$$

Defining now the **density matrix** ρ for a pure state as

$$\rho = |\psi >< \psi| \tag{2}$$

we may rewrite the expectation value of A with the help of the trace-operation as

$$< A >= Tr(\rho A) \tag{3}$$

where

$$Tr\ A = \sum_n < n|A|n > \tag{4}$$

with $|n >$ being an arbitrary complete orthonormal set.

A generalization of the density-matrix may be introduced when one has a number of systems or particles being in different states $|\psi_i >, i = 1..N$, with probabilities p_i. The generalized density matrix then can be written as

$$\rho = \sum_i p_i\ |\psi_i >< \psi_i| \tag{5}$$

again with possibility to take expectation values as in eq.(3). The initial eq.(2) obviously is a special case of this more general density matrix ρ (also called **statistical**

operator), when only one $p_i = 1$ is nonzero. This density-matrix is also called the density-matrix for mixed states. While for a pure state we have $Tr(\rho^2) = 1$, a mixed state is defined by $Tr(\rho^2) < 1$.

Now consider two systems, 1 and 2, for example 1 being a particle and 2 being the whole environment. When these systems are completely uncoupled one may define a product wavefunction

$$|\psi> = |\psi_1> |\psi_2> \tag{6}$$

Let us represent the wavefunctions as an expansion of an orthonormal set

$$|\psi_1> = \sum_n c_n^1 |u_n> \tag{7}$$

$$|\psi_2> = \sum_m c_m^2 |w_m> \tag{8}$$

where index 1,2 represent the two systems, resulting in

$$|\psi> = (\sum_n c_n^1 |u_n>)(\sum_m c_m^2 |w_m>), \tag{9}$$

$$= \sum_{n,m} c_{n,m} |u_n> |w_m> \tag{10}$$

with expansion coefficients $c_{n,m}$. This holds for the two systems 1 and 2 eq.(9) being uncoupled. (Note, however, that the form (10) still represents a pure state but in principle is more general than (9)!)

The density-matrix of the uncoupled systems eq.(9)+(10) is by definition

$$\rho = \sum_{k,l} \sum_{n,m} c_{k,l} c_{n,m}^* |u_k> |w_l>< u_n| < w_m| \tag{11}$$

We now assume that system 2 (the environment) is so large that we cannot obtain sufficient information. In other words we must take an expectation value over that sub-system 2 to obtain a reduced density-matrix ρ_1

$$\rho_1 = Tr_2(\rho) = \sum_r < w_r| \sum_{k,l} \sum_{n,m} c_{k,l} c_{n,m}^* |u_k> |w_l>< u_n| < w_m||w_r> \tag{12}$$

Note that $< w_r||w_l >= \delta_{r,l}$ etc.

This gives explicitly

$$\rho_1 = Tr_2(\rho) = \sum_{k,n} (\sum_r c_{k,r} c^*_{n,r}) |u_k >< u_n| \tag{13}$$

Alternatively we may assume that the two systems are coupled, as the environment 2 may influence the particle 1. A simple example for such a coupling is the following wavefunction

$$|\psi > \; = \; \sum_n c_n |u_n > |v_n > \tag{14}$$

where each eigenfunction $|u_n >$ of the 1 -system is coupled to the eigenfunction $|v_n >$ of the 2 -system.

Performing the same operation as above for the coupled system (14), one obtains the density-matrix

$$\rho = |\psi >< \psi| = \sum_{n,m} c^*_m c_n |u_n > |v_n >< u_m| < v_m| \tag{15}$$

Taking again the trace over the environment (system 2) one has

$$\rho_1 = Tr_2(\rho) = \sum_r < v_r| \sum_{n,m} c^*_m c_n |u_n > |v_n >< u_m| < v_m||v_r > \tag{16}$$

This gives explicitly

$$\rho_1 = Tr_2(\rho) = \sum_r c^*_r c_r |u_r >< u_r| \tag{17}$$

Comparing the reduced density-matrices for the uncoupled case (13) with the coupled case (17), we see that in the uncoupled case the density matrix has off-diagonal terms $k \neq n$, while in the case where the environment is coupled to the system 1 under consideration, the density matrix has diagonal terms only. This coupled case corresponds to a statistical average (5) which means a pure addition of probabilities like for a classical system: *The cat is either dead or alive, not both anymore at the same time.*

A slightly more general model than eq.(14) finally may be defined as follows. Assume that we have a quantum particle S1 with possible eigenstates $|u_n >, n = 1..N$, interacting in the measurement process with an external system S2a described by an equivalent number of degrees of freedom $|v_n >, n = 1..N$, which again is embedded into an even larger environment S2b with $|w_m >, m = 1..M$, and a very large number $M >> N$ of degrees of freedom. This model may be interpreted as follows. The external system S2 represents a measuring instrument which may show macroscopically readable values $|v_n>$ for the corresponding quantum-states $|u_n>$. An example may be the Stern-Gerlach experiment, where the two possible eigenvalues spin-up or spin-down can be observed macroscopically by the deflection of the original electron beam S1 into two different spots in system S2a. In principle it would be sufficient, that the states $|v_n>$ would not overlap. For simplicity of the model we assume here directly that they form a complete orthonormal set. Since this does not yet describe all possible degrees of freedom of the instrument, those other degrees of freedom not directly coupling to the eigenvalues of system S1 are expressed by the states of S2b.

A pure state $|\psi>$ of this combined system now may be defined by our model as

$$|\psi> = \sum_n c_n |u_n> |v_n> \sum_m d_m |w_m> \quad (18)$$

$$= \sum_{n,m} c_n d_m |u_n> |v_n> |w_m> \quad (19)$$

Comparing this with eqs.(14) and (10) we recover the coupling between S1 and S2a, and the uncoupled product between the systems S2b and S2a+S1, as d_m does not depend on n.

The density-matrix becomes explicitly

$$\rho = |\psi><\psi| \quad (20)$$

$$= \sum_{n,m} \sum_{k,l} c_n c_k^* d_m d_l^* |u_n> |v_n> |w_m>< u_k| < v_k| < w_l| \quad (21)$$

Taking the trace first over S2b (or $|w_s>$) gives as in eq.(12) the reduced density-matrix

$$\rho_1 = Tr_w(\rho) \quad (22)$$

$$= \sum_s < w_s| \sum_{n,m} \sum_{k,l} c_n c_k^* d_m d_l^* |u_n> |v_n> |w_m>< u_k| < v_k| < w_l||w_s> \quad (23)$$

$$= (\sum_s d_s d_s^*) \sum_{n,k} c_n c_k^* |u_n> |v_n>< u_k| < v_k| \quad (24)$$

The second trace over S2a (or $|v_r>$) just like in eq.(16) leads to

$$\rho_2 = Tr_v(\rho_1) \quad (25)$$

$$= \sum_r < v_r|(\sum_s d_s d_s^*) \sum_{n,k} c_n c_k^* |u_n> |v_n>< u_k| < v_k||v_r> \quad (26)$$

$$= (\sum_s d_s d_s^*) \sum_r c_r c_r^* |u_r>< u_r| \quad (27)$$

And with $\sum_s d_s d_s^* = 1$ one has the final result

$$\rho_2 = \sum_r c_r^* c_r |u_r >< u_r| \tag{28}$$

which is again a density matrix for a mixed state given in diagonal form, since its matrix elements $< u_k|\rho_2|u_l >$ are nonzero only for $l = k$. The coefficients $c_r^* c_r = |c_r|^2 = p_r$ are the probabilities, to find system S1 in state $|u_r >$ after it has undergone an interaction with system S2=S2a+S2b, where S2 represents a measuring apparatus and/or a large environment.

The unperturbed system, where there is no coupling from the environment, shows **interference** or **coherence** between the possible states through the **off-diagonal** terms, while the reduction to diagonal form of the density matrix occurs through coupling to a (large) system which we can only treat by some averaging procedure as expressed through the traces taken over that second system. This process is called **decoherence** and marks the transition from the quantum-mechanical scale to classical scales.

As an example for such a decoherence-process, the scattering of a quantum particle at a dust particle of diameter a can be described as (E. Joos, in J. Audretsch, editor, *Verschränkte Welt*,Wiley-VCH 2002)

$$\rho(x, x'; t) = \rho(x, x'; 0)\ exp(-\Lambda t(x - x')^2) \tag{29}$$

with $|x - x'|$ the resolution of the microscope, and the localization rate Λ

$$\Lambda \approx a^2 k^2 \frac{Nv}{8\pi^2 V} \tag{30}$$

in units of particles per time and scattering-area. Here k is the wavenumber of incoming particles, a^2 the so-called scattering cross-section, Nv/V the flux-density of the scattered particles. Quantitative examples are a dust-particle with $a = 10^{-5}cm$ as scatterer for cosmic background radiation $\Lambda \approx 10^{-6}cm^{-2}s^{-1}$, sunlight $\Lambda \approx 10^{+17}cm^{-2}s^{-1}$, or molecules of the air $\Lambda \approx 10^{+32}cm^{-2}s^{-1}$. This indicates that in the latter two cases initially existing coherence is destroyed extremely fast. Whether an object shows quantum interferences or not, therefore, is a quantitative question. This also explains, why Schrödingers cat would behave as a classical object, as expected.

(H. Müller-Krumbhaar; for more details see e.g. F. Schwabl, "Quantum Mechanics", Springer-Verlag, Berlin, New York, 2007)