Chapter 2

Does Decoherence Make Quantum Mechanics Coherent?

Measurement, decoherence and the emergence of classical behaviour: which questions decoherence theory answers and which it does not.

Last Update: 19/5/15

1. What is decoherence?

Decoherence theory is two things. It is an attempt to address some of the issues raised by the measurement problem and the classical limit of quantum mechanics. But it is also a procedure for the practical calculation of decoherence. As regards the former it is significantly enlightening but not the whole solution to the problem. However, as regards calculations of decoherence times, or determining what states may be robust against decoherence, it is indispensible. This chapter introduces decoherence at an elementary level and discusses its relevance to measurement and the classical limit following the approach of Zurek (1982,1991) The calculation of decoherence times is illustrated later in Chapter 22 and we shall have more to say about pointer states in Chapter 24.

What do we mean by decoherence? Intuitively it is often imagined to be the disappearance of properties characteristic of quantum mechanical behaviour: the vanishing of the weirdness. But this will not do. Atomic electrons retain indefinitely their discrete energy states, which is essentially quantum mechanical. Moreover, electrons in such states are not localised, which is pretty weird. More specifically, delocalisation causes a quantum state which is initially in a superposition of states, such as,

$$|\psi\rangle = \alpha|a\rangle + \beta|b\rangle \qquad (1)$$

to become either $|a\rangle$ or $|b\rangle$. One signature of this may be that a system looses the ability to produce interference effects, for example. Such effects result from the system being in a superposition state, like (1).

The similarity with quantum measurement theory is immediately apparent. Suppose that $|a\rangle$ and $|b\rangle$ are orthogonal eigenstates of some observable, $\hat{Q}$. After exposing the system in state (1) to an apparatus which measures $\hat{Q}$, the system is left in either state $|a\rangle$ or $|b\rangle$, no longer a superposition. So is decoherence just another name for measurement? No, decoherence theory provides a framework within which measurement can be understood a little better but it is more general, applying also to situations which are not measurements.

A central, unresolved, problem in quantum mechanics is the “collapse of the wavefunction” as the transformation $\alpha|a\rangle + \beta|b\rangle \to |a\rangle$ or $\alpha|a\rangle + \beta|b\rangle \to |b\rangle$ is called. It is indeterminate which of these two outcomes will occur (assuming α and β are both non-zero). In the Copenhagen interpretation of quantum mechanics, states evolve in time according to the Schrodinger equation, $\hat{H}|\psi\rangle = i\hbar\frac{\partial}{\partial t}|\psi\rangle$, except during special events called ‘measurements’ when this irreversible collapse of the wavefunction occurs. Schrodinger (1952) had a great deal of trouble accepting that there was a completely different dynamic operative on special occasions denoted as measurements – and so do most people. Decoherence theory provides a partial clarification by involving the environment (of which the apparatus forms part). The collapse of the system's wavefunction is attributed to the interaction with an environment whose precise quantum state is unknown. This provides insight into the mechanism of wavefunction collapse, and a practical calculational tool, but the measurement problem is not fundamentally solved. Instead it is pushed down one level, into the environment.

2. How does decoherence happen?

Decoherence typically consists of replacing a coherent superposition like (1) with a classical mixture described by the density matrix,

$$(\rho)=\begin{pmatrix} |\alpha|^2 & 0 \\ 0 & |\beta|^2 \end{pmatrix} \tag{2}$$

Prior to decoherence the pure quantum state, (1), could equivalently be described by the density matrix,

$$\hat{\rho}=|\psi\rangle\langle\psi| \Rightarrow (\rho)=\begin{pmatrix} |\alpha|^2 & \alpha\beta^* \\ \alpha^*\beta & |\beta|^2 \end{pmatrix} \tag{3}$$

Now if a measurement in the (a,b) basis is carried out, the pure quantum state (1), or equivalently the density matrix (3), yields the result a with probability $|\alpha|^2$ and the result b with probability $|\beta|^2$. But exactly the same is true of the classical mixture described by the density matrix (2). The classical mixture, (2), differs from the pure quantum state, (3), in the absence of the off-diagonal terms. It is these off-diagonal terms, or cross-terms, which give rise to interference phenomena. The off-diagonal terms produce the magic, and these have gone from (2) – it has decohered.

But how does this decoherence happen? According to decoherence theory, systems are never truly isolated in practice. There is always some interaction with their environment. Suppose the environment starts in some state $|e\rangle$. The state of the environment can change due to its interaction with the system. Thus, if the system were in state $|a\rangle$ the environment would evolve into, say, state $|e(a)\rangle$, whereas if the system were in state $|b\rangle$ the environment would evolve into, say, state $|e(b)\rangle$. Now these changes take place in accord with the Schrodinger equation, i.e., they are unitary in nature. For state (1) the combined system-plus-environment therefore evolves as follows,

$$|\psi\rangle|e\rangle=[\alpha|a\rangle+\beta|b\rangle]|e\rangle \rightarrow \alpha|a\rangle|e(a)\rangle+\beta|b\rangle|e(b)\rangle \tag{4}$$

The density matrix of the combined system-plus-environment is thus,

$$\hat{\rho}=[\alpha|a\rangle|e(a)\rangle+\beta|b\rangle|e(b)\rangle][\alpha^*\langle a|\langle e(a)|+\beta^*\langle b|\langle e(b)|] \tag{5}$$

How can we describe the system alone, uncluttered by the environment? Because we are not bothered about the state of the environment, we wish to find the expectation value of the above $\hat{\rho}$ with respect to all possible environment states. What we are left with, if we take this average over environment states, is called the reduced density matrix, which describes the system alone. Thus we put,

$$\hat{\rho}^{red} = \sum_e \langle e|\hat{\rho}|e\rangle \tag{6}$$

where the sum extends over some orthonormal set of environment basis states $\{|e\rangle\}$. The act of taking the average over the environment states, as in (6), is referred to as "tracing out the environment" (because it consists of summing all the diagonal elements with respect to the environment states, which is the trace operation).

We shall now assume that the states $|e(a)\rangle$ and $|e(b)\rangle$ are orthogonal. The significance of this will soon become clear. Taking $|e\rangle = |e(a)\rangle$ in the sum (6) gives a contribution $|\alpha|^2 |a\rangle\langle a|$, because other terms derived from (5) are zero when the matrix element $\langle e(a)|.....|e(a)\rangle$ is taken. Similarly when $|e\rangle = |e(b)\rangle$ the contribution to the sum is $|\beta|^2 |b\rangle\langle b|$. And that is all there is since all the other states in the summed set $\{|e\rangle\}$ are orthogonal to $|e(a)\rangle$ and $|e(b)\rangle$. So we get,

$$\hat{\rho}^{red} = |\alpha|^2 |a\rangle\langle a| + |\beta|^2 |b\rangle\langle b| \Rightarrow \left(\rho^{red}\right) = \begin{pmatrix} |\alpha|^2 & 0 \\ 0 & |\beta|^2 \end{pmatrix} \tag{7}$$

So the reduced density matrix is just (2), the decohered density matrix. How has this happened? The interaction with the environment has led to the system and the environment becoming entangled – the state (4), or equivalently (5), is no longer expressible as the direct product of a system state and an environment state. But it is generally the case that when one part of a bipartite entangled state is traced out, what results is a mixture not a pure state.

In the language of information and entropy, the evolution (4) consists of the system sharing information about its state with the environment – because its state becomes imprinted on the environment by virtue of the distinct environment states $|e(a)\rangle$ and $|e(b)\rangle$. But when we trace-out the environment we are wantonly throwing away this information. I say "wantonly", but in practice this information has become too difficult to identify once it has become diluted in a large and complex environment. So really we have no practical choice. This throwing away of information is reflected in the increased entropy of the system. Prior to its interaction with the environment the system was in a pure state and thus had zero entropy. Afterwards, the mixed state, (7), has entropy $-\left\{|\alpha|^2 \log_2 |\alpha|^2 + |\beta|^2 \log_2 |\beta|^2\right\} > 0$ (see Chapter 14 for more on quantum entropy, including what happens to entropy on measurement).

Another way of looking at this is to regard the environment as having carried out a measurement on the system and hence "collapsed its wavefunction". The system is left in either state $|a\rangle$ or state $|b\rangle$, with the usual Born rule probabilities, in accord with (7). But in contrast to simply imposing collapse of the wavefunction by *fiat*, the decoherence viewpoint provides a mechanistic explanation underlying the derivation of (7) from (4-6).

3. The Pointer States

Note that in deriving (7) from (5) we had to assume that the two environment states were orthogonal, $\langle e(a)|e(b)\rangle = 0$. The environment has therefore been assumed to provide a perfect measurement, i.e., a perfect discrimination between the system states $|a\rangle$ and $|b\rangle$. [Incidentally, as will be discussed in Chapter 4, the disappearance of the off-diagonal (cross) terms from (7) due to measurement by the environment is exactly the same as the destruction of an interference pattern by making a "which path" measurement]. In general, $|e(a)\rangle$ and $|e(b)\rangle$ will not be orthogonal and the reduced density matrix in the (a,b) basis will not be (7) but will include off-diagonal terms $\alpha\beta^*\langle e(a)|e(b)\rangle$ and its conjugate. Does this mean that decoherence has not happened? No, it does not, as we shall see next.

Thus far we have glossed over a key point. The initial quantum state, (1), could equally well be expressed in some other orthogonal basis, $|\psi\rangle = \alpha'|a'\rangle + \beta'|b'\rangle$. The unitary transformation which relates these two equivalent descriptions is,

$$\begin{pmatrix} |a'\rangle \\ |b'\rangle \end{pmatrix} = \begin{pmatrix} c & d \\ -d^* & c^* \end{pmatrix} \begin{pmatrix} |a\rangle \\ |b\rangle \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} \alpha' \\ \beta' \end{pmatrix} = \begin{pmatrix} c^* & d^* \\ -d & c \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \tag{8}$$

for any complex c, d obeying $|c|^2 + |d|^2 = 1$. But why should the environment choose to measure the states $|a\rangle$ and $|b\rangle$ rather than $|a'\rangle$ and $|b'\rangle$? The point is that whilst $|\psi\rangle = \alpha|a\rangle + \beta|b\rangle = \alpha'|a'\rangle + \beta'|b'\rangle$ are equivalent descriptions of the pure state, the reduced density matrix derived from the equivalent of (5) in the transformed basis is $\hat{\rho}'^{red} = |\alpha'|^2 |a'\rangle\langle a'| + |\beta'|^2 |b'\rangle\langle b'|$ and this is *not* equal to (7). This may be established by substitution of (8) which shows that $\hat{\rho}'^{red}$ has off-diagonal elements in the original a, b basis, namely the coefficient of $|a\rangle\langle b|$ is $\left\{\left(|\alpha|^2 - |\beta|^2\right)\left(|c|^2 - |d|^2\right) + 4\Re\left(cd^*\alpha^*\beta\right)\right\}cd^*$. Whilst this is zero for the trivial transformations with either $c = 0$ or $d = 0$, it is clear that it will not be zero in general.

Consequently, if $\hat{\rho}^{red}$ is diagonal then in general the density matrix $\hat{\rho}'^{red}$ for any other orthogonal basis will not be diagonal. The effect of the environment on the system must be to select a particular basis out of the myriad possibilities to "decohere into". This special basis is called the pointer basis.

Suppose the environment selects (a', b') as the pointer basis, so that decoherence makes $\hat{\rho}'^{red}$ diagonal, but $\hat{\rho}^{red}$ is not diagonal. It must be that, in the (a,b) basis, $|e(a)\rangle$ and $|e(b)\rangle$ are not orthogonal, because otherwise the diagonal nature of $\hat{\rho}^{red}$ would follow from the argument leading to (7). Conversely, in the pointer basis, $|e(a')\rangle$ and $|e(b')\rangle$ *are* orthogonal. Note that decoherence *has* occurred despite the fact that $\hat{\rho}^{red}$ is not diagonal. Vanishing of the off-diagonal components of the density matrix reliably indicates decoherence only if expressed in the pointer basis.

On reflection, this is just as it should be. What we have referred to here as "the environment" could equally well subsume a real measurement apparatus, as well as the uncontrolled environment. But the pointer basis for measurement equipment is not arbitrary, nor is it prescribed by the system. On the contrary, a measuring device is specially designed to measure a particular quantity. It is the measuring device which determines the preferred basis and hence the particular basis in which the density matrix ends up diagonal. This preferred basis is the eigen-basis of the observable being measured. Thus, a device to measure momentum decoheres the system into the momentum basis, and a device to measure the z-component of spin decoheres into the z-spin basis, not, say, the x-spin basis. This selection of the decoherence basis happens during the unitary evolution given by (4). It happens because the apparatus/environment select those states of the system for which the $|e(a)\rangle$ and $|e(b)\rangle$ are orthogonal. This pointer basis has been described by Zurek (1982,1991) as being "einselected" (environmental interaction selected) by the interaction between the system and the apparatus/environment.

Suppose the interaction Hamiltonian, $\hat{H}_{\text{int}}$, between the system and environment/apparatus dominates the dynamics. Then the eigenstates of $\hat{H}_{\text{int}}$ are approximately stationary states. Moreover, any observable which commutes with $\hat{H}_{\text{int}}$ is therefore a constant of motion and shares the same eigenstates. Hence the eigenstates of $\hat{H}_{\text{int}}$ are the pointer states - see Zurek (1981). This simplest case of einselection is the measurement situation. For example, in a Stern-Gerlach apparatus, if the magnetic field and its gradient are in the z-direction, then $\hat{H}_{\text{int}} = -mz\frac{\partial B_z}{\partial z}\sigma_z$ where m is the particle's magnetic moment and σ_z is the Pauli matrix for the z-spin (assuming a spin ½ particle). Hence the pointer states are the eigenstates of σ_z since this commutes with $\hat{H}_{\text{int}}$, whereas, say, σ_x and σ_y do not.

4. Classical Behaviour

So much for measurement, but what does decoherence theory have to say about the emergence of classical behaviour? In part this is already evident. Decoherence reduces a superposition to a classical mixture described by a diagonal density matrix – albeit in a particular preferred basis. But cannot this happen just as readily for a small system as a large system? Why do large things generally behave classically, rather than exhibiting interference effects, entanglement properties, etc? The answer lies, at least in part, in the readiness, and speed, with which larger objects decohere. As will be illustrated in Chapters 22 and 24, small things – with small mass-energy and describable completely by a small number of integers (quantum numbers) – can be contrived to maintain their coherence for long enough to display their quantum magic. We will see that a key factor controlling how quickly a pure quantum state decoheres is the magnitude of the interaction energy with the environment (V) compared with the *spacing* of the system's energy eigenstates, ΔE. If $V << \Delta E$ then the pointer states will tend to be the energy eigenstates of the isolated system. This was first recognised by Paz and Zurek (1999) and is illustrated for a simple system in Chapter 24. This has the implication that if a system is prepared in one of its energy eigenstates, and if the environmental interaction is weak in the sense that $V << \Delta E$, then the system will remain in an energy eigenstate indefinitely. This may mean that spatial delocalisation persists indefinitely. The state of electrons in atoms and molecules provide an example, with well defined energy but distributed spatially.

In contrast, if $V > \Delta E$ the pointer states will tend to be determined by the nature of the interaction between the system and the environment. The relevance of the size of the object is that a large object has a very large number of degrees of freedom, *N*, and the spacing of the system's energy eigenstates generally decreases steeply as N increases (e.g., $\Delta E \propto 1/N^2$ for some simple systems, see Chapter 26 – *is this always true?*). Consequently large systems are doomed to decohere extremely quickly into classical mixed states devoid of quantum weirdness because $V > \Delta E$ is almost inevitable.

Note the liberal use of phrases like "tends to" and "generally" in the above. The tendency of big things to be classical is not unavoidable. Examples of essentially quantum mechanical behaviour on a macroscopic scale, superconductivity and superfluidity, have been studied experimentally since the early decades of the twentieth century. The achievement of Bose-Einstein condensates is a more recent example. It is increasingly the case that quantum behaviour is being coaxed into the macroscopic range, even now at room temperature, e.g., energy eigenstates which are delocalised between two diamonds of macroscopic size (3mm), Lee et al (2011). It is thought that coherent delocalised states play a part in the efficient collection of light energy in photosynthesis, Panitchayangkoon (2010). Big things behaving quantumly are discussed further in Chapter 50 (*not yet written*).

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