

## Chapter 22

### How the Magic is Lost

#### *Illustrations of Decoherence and Persistent Coherence*

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#### 1. Decoherence

The principles of decoherence were described briefly in [Chapter 2](#). In this Chapter a simple example of a decoherence calculation is presented. The simplest possible case is a two-state system. The system is considered to be in an excited state, but the excitation may reside in either of two sites within the system. The corresponding quantum states of the system are denoted  $|1s\rangle$  and  $|2s\rangle$ , where the ‘s’ means that these are states in which the excitation energy is spatially localised (at sites 1 and 2 respectively). However the system has some internal interaction between the two sites. As a result the states  $|1s\rangle$  and  $|2s\rangle$  are not energy eigenstates of the system. Under suitable circumstances the energy eigenstates may be approximated by,

$$|1\rangle = \frac{1}{\sqrt{2}}(|1s\rangle - |2s\rangle) \quad \text{and} \quad |2\rangle = \frac{1}{\sqrt{2}}(|1s\rangle + |2s\rangle) \quad (1)$$

The corresponding eigen-energies are  $E_1$  and  $E_2$ . Writing the free Hamiltonian of the system as  $\hat{H}_0$  we therefore have,

$$\hat{H}_0|i\rangle = E_i|i\rangle \quad (2)$$

In this energy basis,  $\{|i\rangle\}$ , the free Hamiltonian in matrix notation is just,

$$(H_o) = \begin{pmatrix} E_1 & 0 \\ 0 & E_2 \end{pmatrix} \quad (3)$$

The density matrix for the system may be expressed in either basis,

$$\hat{\rho} = \sum_{i,j} \rho_{ij} |i\rangle\langle j| = \sum_{i,j} \rho_{ij}^s |is\rangle\langle js| \quad (4)$$

so that

$$(\rho^s) = \frac{1}{2} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} (\rho) \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} \quad (5)$$

We shall suppose that the system is prepared in state  $|1\rangle$ , the energy eigenstate with energy  $E_1$ . The quantum ‘magic’ in this example is the delocalisation of the excitation energy between two spatially separated sites (known as an ‘exciton’ state) as expressed by (1). Thus the ‘loss of the magic’, or decoherence, will consist of the energy becoming localised onto one or other of the two sites within the system (in other words the state being reduced to either  $|1s\rangle$  or  $|2s\rangle$ , or more generally a classical mixture of these two possibilities). Note that the initial density matrices in the two bases are,

$$(\rho)_0 = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \quad \text{and} \quad (\rho^s)_0 = \frac{1}{2} \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} \quad (6)$$

the latter following from (5). The non-zero off-diagonal components in the density matrix expressed in the spatial basis,  $(\rho^s)_0$ , are necessary in order that  $|1s\rangle$  and  $|2s\rangle$  combine coherently to produce the eigen-state  $|1\rangle$ . For this reason, the off-diagonal components of a density matrix are often (rather loosely) referred to as the “coherences”<sup>1</sup>. Consequently the signature of decoherence in this example will be the vanishing of the off-diagonal terms in  $(\rho^s)$ . However, it is convenient initially to work in the energy basis.

To evaluate decoherence, a specific environmental interaction must be assumed. Suppose the environment couples to the system via an interaction Hamiltonian which in the unperturbed energy basis is,

$$(H_I) = \begin{pmatrix} 0 & V \\ V & 0 \end{pmatrix} \quad (7)$$

This may be interpreted physically as follows. The system’s two energy eigen-states might possess distinct magnetic dipole moments, perhaps due to opposing alignments of a spin  $\frac{1}{2}$  component in the conventional z-direction. Suppose the environment causes a magnetic field in the x-direction,  $\vec{B} = B\hat{x}$ . The magnetic field couples to the system’s magnetic moment via an interaction energy  $m\vec{B} \cdot \hat{\sigma}$  where  $\hat{\sigma}$  are the Pauli matrices and  $m$  is the magnetic dipole moment of the system. For an x-direction field this is  $mB\sigma_x = \begin{pmatrix} 0 & mB \\ mB & 0 \end{pmatrix}$  which is of the form proposed for  $(H_I)$  with  $V = mB$ .

The eigen-energies,  $\lambda$ , of the system are perturbed by interaction with the environment and are given by,

$$\begin{vmatrix} E_1 - \lambda & V \\ V & E_2 - \lambda \end{vmatrix} = 0 \quad (8)$$

This gives, 
$$\lambda_{\pm} = \left\{ E_1 + E_2 \pm \sqrt{(E_2 - E_1)^2 + 4V^2} \right\} / 2 \quad (9)$$

In the unperturbed energy basis the new (perturbed) eigenstates are, (10)

$$\begin{pmatrix} \alpha \\ \beta \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} \beta \\ -\alpha \end{pmatrix} \quad \text{where,} \quad \alpha = \left[ 1 + \left( \frac{\lambda_- - E_1}{V} \right)^2 \right]^{-1/2} \quad \text{and} \quad \beta = \left[ 1 + \left( \frac{V}{\lambda_- - E_1} \right)^2 \right]^{-1/2}$$

Since, at time  $t = 0$ , the system is prepared in free state  $|1\rangle$ , the initial state can be written,

$$|1\rangle \equiv \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \alpha \begin{pmatrix} \alpha \\ \beta \end{pmatrix} + \beta \begin{pmatrix} \beta \\ -\alpha \end{pmatrix} \equiv \alpha |\tilde{1}\rangle + \beta |\tilde{2}\rangle \quad (11)$$

where the tilde denotes the eigenstates of the system when the environmental interaction is taken into account. But assuming that the potential  $V$  is constant, i.e.,

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<sup>1</sup> “rather loosely” because, in general, even a diagonal density matrix (a classical mixture) can be given off-diagonal terms by a change of basis. So non-zero off-diagonal terms do not automatically ensure that the state has any quantum coherent properties. In this example we are specifically concerned with coherence between spatially localised states, so that  $(\rho^s)$  is in the preferred basis.

that the environment state does not change, then the time evolution of the perturbed eigenstates is just,

$$|\tilde{1}, t\rangle = |\tilde{1}\rangle e^{-i\lambda_- t/\hbar} \quad \text{and} \quad |\tilde{2}, t\rangle = |\tilde{2}\rangle e^{-i\lambda_+ t/\hbar} \quad (12)$$

in accord with the Schrodinger equation. Note that in general the interaction with the system will cause the state of the environment to change, so that  $V$  would not necessarily be constant. However it suffices to assume constant  $V$  for this simple illustration. This means that the time evolution of the initial state, (11), can be written down immediately as,

$$|1, t\rangle = \alpha |\tilde{1}\rangle e^{-i\lambda_- t/\hbar} + \beta |\tilde{2}\rangle e^{-i\lambda_+ t/\hbar} \equiv \begin{pmatrix} \alpha^2 e^{-i\lambda_- t/\hbar} + \beta^2 e^{-i\lambda_+ t/\hbar} \\ \alpha\beta (e^{-i\lambda_- t/\hbar} - e^{-i\lambda_+ t/\hbar}) \end{pmatrix} \quad (13)$$

The corresponding density matrix, in the unperturbed energy basis, is,

$$(\rho) = \begin{pmatrix} \alpha^2 e^{-i\lambda_- t/\hbar} + \beta^2 e^{-i\lambda_+ t/\hbar} \\ \alpha\beta (e^{-i\lambda_- t/\hbar} - e^{-i\lambda_+ t/\hbar}) \end{pmatrix} \begin{pmatrix} \alpha^2 e^{-i\lambda_- t/\hbar} + \beta^2 e^{-i\lambda_+ t/\hbar} \\ \alpha\beta (e^{-i\lambda_- t/\hbar} - e^{-i\lambda_+ t/\hbar}) \end{pmatrix}^+ \quad (14)$$

The off-diagonal element being,

$$\begin{aligned} (\rho)_{12} &= (\alpha^2 e^{-i\lambda_- t/\hbar} + \beta^2 e^{-i\lambda_+ t/\hbar}) \alpha\beta (e^{+i\lambda_- t/\hbar} - e^{+i\lambda_+ t/\hbar}) \\ &= \alpha\beta (\alpha^2 - \beta^2) \left(1 - \cos \frac{\Delta\lambda t}{\hbar}\right) - i\alpha\beta \sin \frac{\Delta\lambda t}{\hbar} \end{aligned} \quad (15)$$

where,

$$\Delta\lambda = \sqrt{(E_2 - E_1)^2 + 4V^2} \quad (16)$$

So far we have assumed a single environment state, as effectively labelled by the interaction potential,  $V$ . Decoherence can arise only due to the involvement of more than one environment state. But this can be evaluated only if sufficient is known about the distribution of environment states. In this case we require the probability density of the interaction potentials,  $p(V)$ , so that the reduced density matrix can be found as,

$$(\rho^{red}) = \sum_V p(V) (\rho) \quad (17)$$

where  $(\rho)$  is given by (14). Note that the  $V$ -dependence of  $(\rho)$  comes from the three parameters  $\alpha, \beta, \Delta\lambda$  due to (10) and (16).

In general many different behaviours might result from the sum (17), depending upon the spectral density,  $p(V)$ , of the environment. However our purpose here is only to show that complete spatial decoherence can occur for a suitable choice of  $V$  and  $p(V)$ . It suffices to assume that the strength of the interaction with the environment, as measured by  $2V$ , is far greater than the separation of the energy levels of the unperturbed system. That is,

$$2V \gg |E_2 - E_1| \quad (18)$$

We then have, from (16),  $\Delta\lambda \approx 2V$ , and (9) implies that  $\lambda_- - E_1 \approx -V$  so that (10) gives  $\alpha \approx \beta \approx 1/\sqrt{2}$ . Hence the off-diagonal component of the reduced density matrix becomes,

$$\left(\rho^{red}\right)_{12} = -\frac{i}{2} \sum_V p(V) \sin \frac{2Vt}{\hbar} \quad (19)$$

For instance, if we assume  $p(V)$  has a flat distribution up to some maximum  $V_{\max}$

then we can replace  $\sum_V p(V) \dots$  with  $\int_0^{V_{\max}} \dots \frac{dV}{V_{\max}}$  which leads to,

$$\left(\rho^{red}\right)_{12} = \frac{i\hbar}{4tV_{\max}} \left[ 1 - \cos\left(\frac{2tV_{\max}}{\hbar}\right) \right] \quad (20)$$

This reduces linear as  $1/t$  and will be small for times larger than a decoherence time scale given roughly by  $t_{dec} = \hbar/V_{\max}$ . Perhaps more realistically we could assume an environment with a Gaussian spectral density, so that the integral is of the form

$\int_0^{\infty} \dots \exp\left\{-\frac{V^2}{V_0^2}\right\} \cdot dV$ . This would then result in,

$$\left(\rho^{red}\right)_{12} \propto \exp\left\{-\left(\frac{V_0 t}{\hbar}\right)^2\right\} \quad (21)$$

implying an even more rapid decay of the coherence once  $t > \hbar/V_0$ . In both cases, though, the decoherence timescale is of the form  $t_{dec} \approx \hbar/V$  for some characteristic strength of the environmental interaction,  $V$ .

Examination of the diagonal terms in (14) when  $\alpha \approx \beta \approx 1/\sqrt{2}$  shows that they are both  $1/2$  plus a cross-term. When summed over  $V$  as in (17) these cross-terms will tend to zero for times longer than the decoherence time, for the same reason that we found  $\left(\rho^{red}\right)_{12} \rightarrow 0$ . Consequently the reduced density matrix of the system in the unperturbed energy basis becomes simply,

$$\text{For } t \gg t_{dec} \quad \left(\rho^{red}\right) \rightarrow \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad (22)$$

The final step is to note that, by virtue of (5), the reduced density matrix of the system in the spatial basis is identical to (22). Hence the spatial coherence – the off diagonal terms - have disappeared. The system is now in a classical mixture of states for which the energy resides at site 1 or site 2. The quantum delocalisation has vanished - decohered.

Warning: do not imagine that decoherence times are always well approximated by the result  $t_{dec} = \hbar/V$  derived for this simple example. Things are not so straightforward in every case. Also, do not imagine that it is usual for the (reduced) density matrix to be diagonal in both the energy basis and the spatial basis. This happens in this very simple example only because of the approximation (18) which leads to  $\alpha \approx \beta \approx 1/\sqrt{2}$  and hence to reduced density matrices which are multiples of the unit matrix.

## 2. Persistent Delocalisation

In the preceding example spatial decoherence to a classical mixture of localised states occurred on a timescale of about  $t_{dec} = \hbar/V$ . The key assumption leading to this

conclusion was that the interaction with the environment was strong compared with the system's energy level spacings, i.e.,  $2V \gg |E_2 - E_1|$ .

Providing that the interaction,  $V$ , with the environment is non-zero, then decoherence will typically occur, perhaps on a timescale of around  $t_{dec} \approx \hbar/V$  (though we emphasise that this is not invariably the case). So a weaker environmental interaction will lead to longer decoherence times. However, decoherence rates tend to be very rapid by human standards, even for very weak interactions, because of the small magnitude of  $\hbar$ . Hence, irrespective of whether  $2V \gg |E_2 - E_1|$  or  $2V \ll |E_2 - E_1|$ , an interaction strength of  $\sim 1$  meV will typically (but not invariably!) cause decoherence in the order of a picosecond.

So does it matter whether we are in the regime  $2V \gg |E_2 - E_1|$  or  $2V \ll |E_2 - E_1|$ ? Yes, it does, but the distinction between these two cases lies in the corresponding pointer states. It turns out that the latter case, the weak environmental interaction, results in pointer states which approximate to the energy eigenstates. Thus, if the initial state is close to an energy eigenstate then decoherence will alter it little, and spatial delocalisation will persist even after decoherence. Atomic electron orbitals are the obvious example. These remain in energy eigenstates and are spatially delocalised permanently as a result.

Our simple example can be used to illustrate how coherence can persist if the interaction with the environment is weak compared with the spacing of the system's energy levels. Thus if,

$$2V \ll |E_2 - E_1| \quad (23)$$

then  $\Delta\lambda \approx |E_2 - E_1|$  and  $\lambda_{\pm} \approx E_1, E_2$  and hence  $\alpha \approx 1$ ,  $\beta \approx 0$ . So (14) gives the density matrix in the unperturbed energy basis to be about  $\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$  at all times, so that in the

spatial basis (5) gives  $(\rho^s) \approx \frac{1}{2} \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}$ . The former means that the initial energy eigenstate persists indefinitely, and the latter is merely a reminder that this implies coherence in the spatial basis (non-zero off-diagonal terms).

Note that it is not merely that decoherence takes a long time. The spatial coherence remains indefinitely (as for atomic electron orbitals) because the pointer states are the energy eigenstates which are spatially delocalised. This can be seen from (14) if we consider  $\beta$  to take some small but non-zero value  $|\beta| \ll |\alpha|$ . Then the density matrix element  $\rho_{11}$  is much larger than the other components of  $(\rho)$  at all times. The exact magnitudes of  $\rho_{ij}$  will oscillate, but  $\rho_{11}$  is always much larger than the other components. Consequently the 'pointer states' resulting from the environmental interaction, and given by  $(\rho)$ , approximate to the energy eigenstates at all times however long.

In fact it can be shown quite generally that if the energy available from environmental interaction is small compared with the *spacings* of the free system's energy levels, then the pointer states approximate to the free system's eigenstates. In [Chapter 24](#) we illustrate this with a further model.

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