

Chapter 24

How the Magic is Retained

If the interaction energies with the environment are small compared with the spacing of the system's eigen-energies then the pointer states towards which the system decoheres are the energy eigenstates. An initial energy eigenstate, and its attendant spatial delocalisation, is then proof against the ravages of decoherence. This is illustrated here using a simple model.

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1. Introduction: The Theorem of Paz-Zurek-Gogolin

In general, interaction with the environment will cause an initially pure quantum state to decohere into a mixed state. In [Chapter 2](#) we saw that each system-environment combination defines a particular set of pointer states, these forming the basis in which the decohered mixed state density matrix is diagonal. If the system-environment interaction energy is small compared with the spacings between the system's free eigen-energies, then the pointer states will approximately coincide with the system's energy eigenstates. This was first recognised and demonstrated in the context of a particular model by Paz and Zurek (1999). The theorem has been proved in all generality recently by Gogolin (2010). Here we merely make the theorem plausible to the reader by illustrating how it arises in a very simple model. The implication is that, if a system is prepared in an energy eigenstate, often spatially delocalised, then this spatial delocalisation will persist indefinitely. On the other hand, if the system starts in some other pure quantum state, then it will decohere into a mixture of energy eigenstates.

At the opposite extreme is the case that the environmental interaction is strong compared with the system's energy level spacings. In this case the pointer states are not the system's energy eigenstates. Instead they approximate to the eigenstates of the interaction Hamiltonian. The general situation is summarised by Paz and Zurek (1999) thus: *“There are three basically distinct regimes in which one can analyze the properties of the pointer states selected through decoherence. They differ through the relative strength of the self-Hamiltonian and of the Hamiltonian of interaction. The first one is the measurement situation where the self-Hamiltonian of the system is negligible and the evolution is completely dominated by the interaction with the environment. In such cases, pointer states are eigenstates of the interaction Hamiltonian. The second, most common and complex situation, occurs when neither the self-Hamiltonian nor the interaction with the environment are clearly dominant. Then the pointer states arise from a compromise between self-evolution and interaction. The third situation corresponds to the case where the dynamics is dominated by the system's self-Hamiltonian. In this case einselection produces pointer states which coincide with the energy eigenstates of the self-Hamiltonian”.*

We now illustrate this last possibility.

2. A Simple Model Illustrating the Theorem of Paz-Zurek-Gogolin

Consider a two-level system with free Hamiltonian \hat{H}_S such that,

$$\hat{H}_S |I\rangle = E_I |I\rangle \quad (1)$$

for $I=1,2$ with $E_1 < E_2$. Suppose the system interacts with an environment such that the interaction Hamiltonian is \hat{V} . The environment states will be denoted $|e\rangle$. The environment is assumed to be in some mixed state given by the density matrix,

$$\hat{\rho}_{env} = \sum_e p(e) |e\rangle\langle e| \quad (2)$$

for real p with $0 \leq p(e) \leq 1$ and $\sum_e p(e) = 1$. If the environment were in the state $|e\rangle$ then

the interaction Hamiltonian acting on the system's sub-space alone is written $\hat{V}(e)$. In this case the system's energy eigenstates are perturbed from their free states by the interaction and are given by,

$$(\hat{H}_S + \hat{V}(e)) |I, e\rangle = E_I^e |I, e\rangle \quad (3)$$

The dependence of the perturbed eigenstates/eigenvalues on the environment state is denoted by the label "e". Suppose the system starts in an arbitrary pure state, which can be expressed in either basis thus,

$$|\psi_0\rangle = \alpha|1\rangle + \beta|2\rangle = \tilde{\alpha}|1, e\rangle + \tilde{\beta}|2, e\rangle \quad (4)$$

where $\tilde{\alpha}, \tilde{\beta}$ will depend upon the environment state, e . We now make the simplifying assumption that the environment states do not change due to the interaction with the system, so that the time evolution of a combined pure state is,

$$|\psi_0\rangle|e\rangle \rightarrow |\psi_t(e)\rangle|e\rangle \quad (5)$$

We have already seen in Chapter 22 that the restriction to a constant environment state, whilst not realistic, does not prevent decoherence. The evolution of the system state, allowing for the interaction with the environment, follows from Schrodinger's equation, $(\hat{H}_S + \hat{V}(e))|\psi_t\rangle = i\hbar \frac{\partial}{\partial t} |\psi_t\rangle$, from which we get,

$$|\psi_t(e)\rangle = \tilde{\alpha} \exp\left\{-i \frac{E_1^e t}{\hbar}\right\} |1, e\rangle + \tilde{\beta} \exp\left\{-i \frac{E_2^e t}{\hbar}\right\} |2, e\rangle \quad (6)$$

The combined system-plus-environment density matrix evolves as,

$$\hat{\rho} = \sum_e p(e) |e\rangle\langle e| \otimes |\psi_0\rangle\langle\psi_0| \rightarrow \sum_e p(e) |e\rangle\langle e| \otimes |\psi_t(e)\rangle\langle\psi_t(e)| \quad (7)$$

The reduced density matrix describing the system alone is obtained by tracing-out the environment,

$$\hat{\rho}_{red} = \sum_{e'} \langle e' | \hat{\rho} | e' \rangle = \sum_e p(e) |\psi_t(e)\rangle\langle\psi_t(e)| \quad (8)$$

The pair of states $\{|1\rangle, |2\rangle\}$ are orthogonal, as are the pair of states $\{|1, e\rangle, |2, e\rangle\}$, because both are eigenstates of an Hermetian Hamiltonian with distinct eigenvalues. So there is a unitary transformation between them, which can be written in terms of some coefficients a, b such that $|a|^2 + |b|^2 = 1$ thus,

$$\begin{pmatrix} |1, e\rangle \\ |2, e\rangle \end{pmatrix} = \begin{pmatrix} a & b \\ -b^* & a^* \end{pmatrix} \begin{pmatrix} |1\rangle \\ |2\rangle \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} \tilde{\alpha} \\ \tilde{\beta} \end{pmatrix} = \begin{pmatrix} a^* & b^* \\ -b & a \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \quad (9)$$

Note that the coefficients a, b depend upon the environment state, e . Substituting (9) into (6) and re-arranging gives,

$$|\psi_t(e)\rangle = \left[(|a|^2 \alpha + ab^* \beta) \exp\left\{-i \frac{E_1^e t}{\hbar}\right\} + (|b|^2 \alpha - ab^* \beta) \exp\left\{-i \frac{E_2^e t}{\hbar}\right\} \right] |1\rangle + \left[(a^* b \alpha + |b|^2 \beta) \exp\left\{-i \frac{E_1^e t}{\hbar}\right\} + (-a^* b \alpha + |a|^2 \beta) \exp\left\{-i \frac{E_2^e t}{\hbar}\right\} \right] |2\rangle \quad (10)$$

Substitution of (10) into (8) yields an expression for the reduced density matrix. However, before doing this it is sensible to simplify (10) for the case that the environmental interaction is weak. By this we mean that the matrix elements of the interaction potential, $\hat{V}(e)$, are small compared with $E_2 - E_1$. This is exactly the condition for which we may employ first order perturbation theory. So we have,

$$b \approx -\frac{V_{21}}{E_2 - E_1} \quad \text{where, } V_{21} = \langle 2 | \hat{V}(e) | 1 \rangle \quad (11)$$

and a is $\sqrt{1 - |b|^2}$. The weak environment condition therefore gives,

$$|V_{21}| \ll |E_2 - E_1| \Rightarrow |b| \ll |a| \approx 1 \quad (12)$$

Hence, retaining only leading terms in (10) we get,

$$|\psi_t(e)\rangle \approx \left[\alpha \exp\left\{-i \frac{E_1^e t}{\hbar}\right\} \right] |1\rangle + \left[\beta \exp\left\{-i \frac{E_2^e t}{\hbar}\right\} \right] |2\rangle \quad (13)$$

Substitution in (8) provides the components of the reduced density matrix in the basis of the unperturbed (free) system's energy eigenstates to be, to first order,

$$(\rho_{red})_{11} = |\alpha|^2 \quad (14a)$$

$$(\rho_{red})_{22} = |\beta|^2 \quad (14b)$$

$$(\rho_{red})_{12} = \alpha \beta^* \sum_e p(e) \exp\left\{i \frac{(E_2^e - E_1^e) \cdot t}{\hbar}\right\} \quad (14c)$$

Recall that α, β are the coefficients in terms of which the arbitrary initial state is expressed in the energy basis, (4). Consequently they are independent of the environment state and can be taken outside the sum over the e states. The energy eigenvalues which appear in (14c) are, however, those of the perturbed states, and hence depend upon the environment state, e . Again first order perturbation theory tells us what these perturbed eigenvalues are, approximately, i.e.,

$$E_1^e \approx E_1 + V_{11} \quad \text{and} \quad E_2^e \approx E_2 + V_{22} \quad (15a)$$

$$\text{where,} \quad V_{11} = \langle 1 | \hat{V}(e) | 1 \rangle \quad \text{and} \quad V_{22} = \langle 2 | \hat{V}(e) | 2 \rangle \quad (15b)$$

Putting $\Delta V(e) = V_{22} - V_{11}$, (14c) becomes,

$$(\rho_{red})_{12} = \alpha \beta^* \exp\left\{i \frac{(E_2 - E_1) \cdot t}{\hbar}\right\} \sum_e p(e) \exp\left\{i \frac{\Delta V(e) \cdot t}{\hbar}\right\} \quad (16)$$

For times which are long compared with $\hbar / \Delta V(e)$ the relative phases of the terms in this sum will differ by amounts which are large compared with unity. Hence, for such times, the sum in (16) is over terms with essentially random relative phases.

Consequently there will be strong cancellation and it is fairly clear that the sum will reduce to zero for $t \gg \hbar / \Delta V(e)$. Explicit evaluation of the sum requires some model for the environment to provide the spectrum of states, $p(e)$. In [Chapter 22](#) we considered a flat spectrum up to some energy cut-off, ΔV_{\max} , and showed that a similar integral reduced to zero $\propto \hbar / \Delta V_{\max} t$. A Gaussian spectrum of width ΔV_{σ} led

to an exponential decay: $(\rho^{red})_{12} \propto \exp\left\{-\left(\frac{\Delta V_{\sigma} t}{\hbar}\right)^2\right\}$.

Consequently, on a timescale $t \gg \hbar / \Delta V$, where ΔV is some characteristic environmental interaction energy, the initial pure state decoheres into a mixed state whose density matrix in the energy basis is,

$$(\rho_{red}) = \begin{pmatrix} |\alpha|^2 & 0 \\ 0 & |\beta|^2 \end{pmatrix} \quad (17)$$

This shows that, for this illustrative example, a weak environmental interaction, such that $|V_{21}| \ll |E_2 - E_1|$, leads to the energy eigenstates being the pointer states, since the density matrix becomes diagonal in this basis at times long compared with $\hbar / (V_{22} - V_{11})$.

One may reasonably ask what is special about the energy basis that this is so? What is special about the energy basis is that time evolution and energy are intimately related. Time evolution is governed by the Hamiltonian, which is also the energy operator. Time and energy are conjugate variables, and energy is that quantity which is conserved due to temporal homogeneity by Noether's Theorem.

Note that, despite the so-called 'weak environment', $|V_{21}| \ll |E_2 - E_1|$, decoherence still occurs in general, and the corresponding timescale (typically, but not always, $\sim \hbar / \Delta V$) may be very short. Interaction strengths in the order of milli-eV produce decoherence in the order of picoseconds if $\hbar / \Delta V$ is indicative. The initial pure state, (4), becomes the mixed state, (17). However, an obvious exception is when the initial state happens to be an energy eigenstate, say $|1\rangle$ with $\alpha = 1, \beta = 0$. Then (4) and (17) are identical. There is no decoherence because the initial state happens to be a pointer state. Moreover, since an energy eigenstate will generally be spatially delocalised, this delocalisation will persist indefinitely. If the quantum magic is associated with this delocalisation (for example because it produces some interference phenomenon) then the magic will persist indefinitely.

A possible example of this are the recent measurements of sustained coherence in photosynthetic systems, e.g., Engel et al (2007) and the references cited in Bradford (2011). Quoting Engel et al (2007), "*Photosynthetic complexes are exquisitely tuned to capture solar light efficiently, and then transmit the excitation energy to reaction centres, where long term energy storage is initiated. The energy transfer mechanism..... invokes 'hopping' of excited-state populations along discrete energy levels.....spectroscopic data clearly document the dependence of the dominant energy transport pathways on the spatial properties of the excited-state wavefunctions of the*

whole bacteriochlorophyll complex..... electronic quantum beats arising from quantum coherence in photosynthetic complexes have been predicted and indirectly observed. Here we extend previous two-dimensional electronic spectroscopy investigations of the FMO bacteriochlorophyll complex, and obtain direct evidence for remarkably long-lived electronic quantum coherence playing an important part in energy transfer processes within this system. The quantum coherence manifests itself in characteristic, directly observable quantum beating signals among the excitons within the Chlorobium tepidum FMO complex at 77 K. This wavelike characteristic of the energy transfer within the photosynthetic complex can explain its extreme efficiency, in that it allows the complexes to sample vast areas of phase space to find the most efficient path.”

The longevity of the observed quantum beats exceeded expectation prior to 2007. The point here is that the “warm, wet” environment in biological systems is normally considered to create a strong interaction with the organelle, and hence to imply very rapid decoherence. It is feasible that the explanation for the observed sustained spatial coherence is simply that the interaction between neighbouring chromophores is strong, resulting in exciton energy level spacings which exceed the energies available in the environment. In this case spatial coherence would be maintained despite the potential for rapid decoherence because the pointer states are the energy eigenstates, and so an initial energy eigenstate (exciton) would be unaffected by decoherence. The case for this has been argued by Bradford (2011).

References

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