Decoherence within a simple Model for the Environment

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Abstract

This article examines the decoherence of a macroscopic body using a simple model of the environment and following the evolution of the pure state for the whole system. We found that decoherence occurs for very general initial conditions and were able to confirm a number of widely accepted features of the process.

Key words: Decoherence, reduced density matrix, preferred basis, macrosuperpositions.
1. INTRODUCTION

There is growing interest in decoherence, particularly as it promises to deepen our understanding of the macroscopic world in terms of quantum principles [1]. If we suppose that $B$ is a macroscopic body (say a point particle with a very large mass $M$ and position co-ordinate at the centre of mass) interacting with an environment $E$, we know from a host of examples that if we start with a factorized state of the two systems, the environment state vectors associated with the body’s distinct positions (at least macroscopically) rapidly become orthogonal to each other, irrespective of the initial conditions. The spatial correlations of $B$, whose reduced density matrix becomes diagonal on a position basis, are suppressed by decoherence. Thanks to this apparent collapse due to interaction with the environment, we see the classic characteristics of the macroscopic world emerge. During the above mentioned process temporal evolution also affects body $B$. In a number of examples, however (some in a seminal paper by Joos and Zeh [2]), wave packet spreading is ignored. This is justified both by the speed of the decoherence process and because mass $M$ is large. We will adopt this approximation by formally ignoring the term of the body’s kinetic energy in the total Hamiltonian. This is rigorous with the limiting condition that $M$ is infinite. Realistic sources of decoherence are described in the literature on the subject, such as scattering [2, 4] and quantum gravity [4, 5] but the focus is generally on useful and practical models such as the so-called Caldeira-Legett environment [7], which in any case reflects certain physical situations. Omnes [8] recently put forward a general theory of the decoherence effect encompassing both Caldeira-Legett’s harmonic model and the external environment considered by Joos and Zeh [2], as well as being related to the quantum state diffusion model [9]. In the applications mentioned, the usual approach is to study the temporal evolution of the reduced density matrix we are interested in, which obeys an irreversible master equation [10]. Resorting to this technique is almost inevitable as the overall system has many (or infinite) degrees of freedom. However, in my opinion at least, it would be useful to propose a further example of decoherence within the framework of an environment model using Schrödinger evolution of the initial pure state. Since the seminal paper by H. D. Zeh, published in the very first issue of Foundations of Physics [11], our understanding of the decoherence process has gradually
shifted from qualitative to quantitative. Our aim is to use pure state evolution to obtain analytical results independent of a particular master equation. While there will be no ground breaking results, a new example could provide a further confirmation of our convictions, as well as offering a number of points worthy of consideration. This means the paper is didactic to a certain degree, but also represents a small step forward in our understanding of the decoherence process in quantitative terms.

2. THE MODEL FOR THE ENVIRONMENT

The example we will discuss concerns a one dimensional system in which the external environment is represented by \( n \) identical particles with \( x \) axis co-ordinates \( x_1, x_2, \ldots, x_n \). The macroscopic body’s position is indicated by \( X \). The Hamiltonian for the environment is based on the Hepp-Coleman\(^\text{[12]}\) model, which appeared some time ago and was also discussed by Bell\(^\text{[13]}\). It was used to discuss the problem of measurement in terms of apparent collapse. (It was actually adopted to describe the system to observe, whereas here it will be used to describe the environment which acts as observer). The model considers the particle’s kinetic energy as proportional to its momentum rather than as given by the customary quadratic term. The wave packet of a free particle of this sort moves along the axis in a single direction without changing form. Our Hamiltonian for the environment is

\[
H_e = \alpha \sum \hat{p}_i + V(x_1, x_2, \ldots, x_n) \tag{1}
\]

where \( \hat{p}_i \) is the momentum, \( \alpha \) is a constant quantity with the dimension of velocity, and the potential term \( V(x_1, x_2, \ldots) \) includes both one particle interactions and two or many particle interactions. The expression assumed for the kinetic term is rather unconventional and the hamiltonian is considered to be an appropriately idealized toy model. However, the intuition can be supported by reference to physical models. In the case of a free particle, for example, it may be considered as the caricature of an electron in one dimensional motion. Let us consider the ultra-relativistic approximation frequently used for very energetic electrons, and which amount to take the rest mass to be zero in Dirac equation. Then this transform \(^\text{[14]}\) in a couple of Weyl equations given by the hamiltonians \( H_\pm = \pm c \sigma \cdot \hat{p} \) applied to a two component spinor. As usual \( \sigma \) denotes the Pauli matrix in vectorial form.
Considering $H_-$ and assuming that the spin of each particle in the one dimensional system is antiparallel to the $x$ axis (i.e. by considering only the component with $S_x = -1/2$ for all particle spinors) we obtain the kinetic part of $H_e$, with $\alpha = c$. The free waves with positive momentum represent a massless particle with spin pointing in the opposite direction (a neutrino). The free waves with negative momentum, on the other hand, have negative energy and opposite helicity and should be referred to as antiparticles. The problem now is the other term in our environment Hamiltonian, as it is not easy to imagine an interaction depending on positions, which in any case should be given in a relativistically correct form for particles of this type.

We may also consider the electrons in the periodic field of crystal atoms, which may be thought of as free ”dressed electrons”. We know[15] that for an infinite simple cubic lattice the one dimensional motion energy curves of these free ”quasi particles” can be described with a good degree of accuracy in the form:

\[ W(n) = A_n - B_n \cos(aq) \]

where $a$ is the lattice spacing and $q$ the reduced wave vector. Interest is usually focused on the neighbours at the top and bottom of the band. But for our purposes we take one band (for example the first) and develop the dispersion relation above near $qa = \pi/2$, assuming the zero of energy scale to be $A_0$:

\[ W(q)_0 - A_0 = B_0(aq - \pi/2) = B_0aq' = E(q') \]

with the limitation $|aq'| < 1$. We then follow Wannier’s method[16] and replace $q'$ with $-id/dx$ in the last expression to obtain the effective Hamiltonian:

\[ H = E(-id/dx) = (B_0a/\hbar)\hat{p} \]

Our model can therefore be thought of as describing a one dimensional system of interacting quasi particles in a limited pseudo-momentum zone.

For the interaction of the environment with body $B$ we will assume the linear coupling $W^{(sc)} = kX \sum x_i$, where $k$ is a constant, already considered in the literature. It is similar, for example, to von Neumann’s measurement interaction[17]. This coupling is debatable in that it is not invariant under translation[18]. For our purposes we will use it in this form, but will then show that it can safely be replaced by a harmonic coupling. If we assume $B$ is free (apart from interaction with the environment) and use the approximation
mentioned above for a very large $M$, we can write the total Hamiltonian as $H = H_e + W^{(sc)}$. We will let

$$\chi_0 = \psi(X) \varphi(x_1, x_2, \ldots)$$

be the initial state. We are interested in its time evolution and since the commutator $[H_e, W^{(sc)}]$ of the two terms appearing in the total Hamiltonian commutes with both, we can write:\[13\]:

$$\chi_t = e^{-itH_e/\hbar} e^{-itkX} e^{i\alpha kX t^2/\hbar^2} \psi(X) \varphi(x_1, x_2, \ldots) \ . \quad (2)$$

We now replace $W^{(sc)}$ with the coupling $W^{(mc)} = \gamma \hat{P} \sum x_i$, where $\hat{P}$ is the momentum operator of $B$ and $\gamma$ is a constant. By following a similar path it is easy to write $\chi_t$ on momentum basis of the macroscopic body:

$$\chi_t = \tilde{\psi}(P) e^{i\alpha \gamma P t^2/\hbar^2} e^{-itH_e/\hbar} e^{-it\gamma P} \sum x_i/\hbar \varphi(x_1, x_2, \ldots, x_n) \quad (3)$$

where $\tilde{\psi}(P)$ is the Fourier transform of $\psi(X)$. In the case of coupling $W^{(sc)}$ we will also consider the generic entangled initial state $\Phi(X, x_1, x_2, \ldots, x_n)$. In this case:

$$\chi_t = e^{i\alpha kX t^2/\hbar^2} e^{-itH_e/\hbar} e^{-itkX} \sum x_i/\hbar \Phi(X, x_1, x_2, \ldots, x_n) \ . \quad (4)$$

We will use these equations later.

### 3. THE REDUCED DENSITY MATRIX

We will first consider the case of coupling $W^{(sc)}$ and calculate the macroscopic body’s reduced density matrix elements $\rho^{(sc)}_{X'X''}$ on the position basis. They are obtained by taking a partial trace of the total density matrix, i. e. integrating $\langle X' | \chi_t | X'' \rangle$ over all the degrees of freedom of the environment:

$$\rho^{(sc)}_{X'X''} = \psi(X') \psi^*(X'') e^{i\alpha k(X' - X'') t^2/\hbar^2} \int dx_1 \cdots dx_n \varphi^*(x_1, \ldots, x_n) \varphi(x_1, \ldots, x_n) e^{itk(X' - X'')} \sum x_i/\hbar \ . \quad (5)$$

We used Eq. (2) and the fact that operator $A = e^{itH_e/\hbar}$ is unitary.
The above equation can be further manipulated by introducing, in lieu of $x_i$ the co-ordinate $\eta = \sum x_i/n$ of the centre of mass of the particle system constituting the environment and the co-ordinates of the particles with respect to their centre of mass: $x_i = \eta + \xi_i$. The $\xi_i$ are not independent as they must satisfy the relation $\sum_{i=1}^{n} \xi_i = 0$. We will consider $\eta$ and the first $n - 1$ relative co-ordinates (i.e. $\xi_1, \xi_2, \cdots, \xi_{n-1}$) as independent variables. The last relative co-ordinate is expressed as $\xi_n = - \sum_{i=1}^{n-1} \xi_i$. The Jacobian determinant of the transformation is equal to $n$. We will write the integration volume element for the new variables as $dV = d\eta dS$, where $dS = n d\xi_1 d\xi_2 \cdots d\xi_{n-1}$. By integrating $\varphi^*(\eta + \xi_1, \cdots) \varphi(\eta + \xi_1, \cdots)$ as expressed in the new variables on $dS$ and keeping $\eta$ fixed, we obtain the quantity

$$w(\eta) = \int dS \varphi^*(\eta + \xi_1, \cdots) \varphi(\eta + \xi_1, \cdots)$$  \hspace{1cm} (6)

which is the probability density distribution of $\eta$ in the initial state. If we define $z = nk(X' - X'') t / \hbar$ we obtain

$$\rho^{(sc)}_{X'X''} = \psi(X') \psi^*(X'') e^{i \alpha k (X' - X'') t^2 / \hbar^2} \int d\eta e^{iz\eta} w(\eta) .$$  \hspace{1cm} (7)

The Fourier transform $f(z) = FT[w(\eta)] = \int d\eta e^{iz\eta} w(\eta)$ therefore appears as a factor in the expression of $\rho^{(sc)}_{X'X''}$. In passing we note that at each successive instant, as is apparent from the previous expression, the absolute values of the off diagonal matrix elements can never be bigger than their initial values. If we consider the mean value $\overline{\eta}$ of $\eta$, and its mean square deviation $\sigma = (\eta - \overline{\eta})^2$ (which we take as finite), for short periods of time we obtain:

$$|f(z)| = (1 - \sigma z^2 / 2) .$$  \hspace{1cm} (8)

Now, as $w(\eta)$ is a positive definite quantity with mean square deviation $\sigma \geq 0$, in the initial moments the absolute value of the off diagonal matrix elements decreases, apart from the exceptional case in which $\sigma = 0$. But the really interesting point is the asymptotic time behaviour. Here we see not only that $w(\eta)$ is a real definite positive function, but also that its integral extended from minus to plus infinity must be one. So when we have an ordinary function, it is absolutely integrable, with the result that $|f(z)| \to 0$ for $z \to \pm \infty$. This brings us to the important conclusion that starting from any factorized initial state, the off diagonal matrix elements $\rho^{(sc)}_{X'X''}$ (excluding exceptional
cases) go asymptotically to zero in the two time directions. To this end we should remember that if $w(\eta)$ is $m$ times continuously differentiable and its $m$ derivatives are integrable, we obtain $|f(z)| \to 0$ for $z \to \pm \infty$ more quickly than $1/z^m$. If $w(\eta)$ is one of the more commonly encountered probability density distributions (such as a Lorentz or a Gaussian distribution), the off diagonal matrix elements tend to zero like the related Fourier transform, an exponential or a Gaussian, respectively. When the environment initial state vector is factorized in the states of the individual components, the probability distribution $w(\eta)$ is a Gaussian under very general and physically acceptable conditions.

Additional insights into the result obtained above are provided by the following examples, which consider the unfavourable case of a non differentiable function such as

$$w(\eta) = \begin{cases} 
1/2L & \text{if } |\eta| < L \\
0 & \text{otherwise}
\end{cases}$$

and the case in which $w(\eta)$ is a non-ordinary and somewhat singular “function” such as a $\delta(\eta - \bar{\eta})$. In the first case we have

$$f(z) = \sin[zL]/zL = \sin[nk(X' - X'')Lt/\hbar]/[nk(X' - X'')Lt/\hbar] \quad (9)$$

which allows us to define a decoherence time scale $\tau^{(sc)} = \hbar/[nk(X' - X'')\Delta \eta]$, where $\Delta \eta$ is the width of $w(\eta)$. In the second we have

$$f(z) = e^{iz\pi}.$$ 

As we can see, the absolute value $\rho^{(sc)}_{X'X''}$ is now a constant of motion but in spite of this the phase oscillations, which get increasingly faster, might help towards practically cancelling out the spatial correlations. So far we have assumed that environment wave function $\varphi(x_1, x_2, \ldots, x_n)$ is normalizable in the usual sense (especially with respect to the variable $\eta$), i.e. as a square integrable wave function. But we also have to consider the case in which, for instance, the state of $\eta$ is that of a pure plane wave. In these circumstances we could resort to box normalization and obtain our result simply by taking the limit for $L$ going to infinity in Eq. (9). In this case decoherence is immediate.

We will now consider the case of linear coupling $W^{(mc)}$ rather than coupling $W^{(sc)}$. Using Eq (3) and following, mutatis mutanda, the steps we took before, we now see that the off diagonal elements $\rho^{(mc)}_{P'P''}$ of the macroscopic
body's reduced density matrix on the momentum basis depends on time as:

\[
\rho^{(mc)}_{P'P''} = \bar{\psi}(P')\bar{\psi}^*(P'')e^{in\alpha\gamma(P' - P'')t^2/\hbar^2}\int d\eta e^{iy\eta}w(\eta)
\]  

(10)

where \(y = n\gamma(P' - P'')t/\hbar\). The value of \(|\rho^{(mc)}_{P'P''}|\) (as is the case for \(W^{(sc)}\) interaction) depends on the Fourier transform \(f(y) = FT[w(\eta)]\), which means that time behaviour is the same as in the previous case, replacing \(z\) with \(y\).

The results we obtained for both couplings have a very plausible interpretation. Looking at Eq (2) and Eq (3) we see that the initial state of the environment, coupled respectively to \(X'\) and \(X''\) (Eq (2)) or to \(P'\) and \(P''\) (Eq (3)), simply move apart in Hilbert space (actually in both directions of time). Indeed

\[e^{itkX'\sum x_i/\hbar}\varphi(x_1, x_2, \ldots)\]

gives a momentum translation amounting to \(tkX'\) for each particle of the environment, i.e. to \(tkX'n\) for their centre of mass (c.m.). The two wave packets of the c.m. (coupled to \(X'\) and \(X''\) or to \(P'\) and \(P''\) respectively) then become separate on a momentum basis by the quantity \(tk|X' - X''|n\) (or \(t\gamma|P' - P''|n\)) and at some time no more overlap. If the mean square deviation of the environment's c.m. momentum is denoted as \(\Delta\pi\), we may suppose that decoherence is established after a time \(\tau^{(sc)} = \Delta\pi/kn|X' - X''|\) (or \(\tau^{(mc)} = \Delta\pi/\gamma n|P' - P''|\) respectively). We may use the indeterminacy relation to write \(\tau^{(sc)} = \hbar/kn|X' - X''|\Delta\eta\), thus recovering the definition already given of a "decoherence time" scale.

Let's go back to the spatial coupling \(W^{(sc)}\) and take a generic wave function \(\Phi(X, x_1, x_2, \ldots, x_n)\) as the initial state. We assume it is square integrable and continuous with continuous first derivatives for all variables. Using Eq (4) we obtain:

\[
\rho^{(sc)}_{X'X''} = e^{in\alpha k(X' - X'')t^2/\hbar^2}g(z)
\]  

(11)

where \(g(z) = FT[w_{X'X''}(\eta)]\), with an obvious extension of the notation, is the Fourier transform of:

\[w_{X'X''}(\eta) = \int \Phi(X', \eta + \xi_1, \ldots, \eta - \sum_{i=1}^{n-1} \xi_i)\Phi^*(X'', \eta + \xi_1, \ldots, \eta - \sum_{i=1}^{n-1} \xi_i)dS
\]  

(12)

The co-ordinates transformation thus introduced does not affect the assumed square integrability or the analytical properties of the initial state wave function expressed in the new variables. Evidently \(w_{X'X'}(\eta) = |w_{X'X'}(\eta)|\) and
\[ w_{X''X'}(\eta) = |w_{X''X'}(\eta)| \] are absolutely integrable in \( \eta \), and therefore their square root will be square integrable. If we apply Schwarz inequality to the integration in \( dS \), we obtain

\[ |w_{X''X'}(\eta)| \leq w_{X''X'}^{1/2}(\eta)w_{X''X'}^{1/2}(\eta). \]  \hspace{1cm} (13)

The right hand quantity is integrable in \( \eta \), as is clear if we again apply Schwarz inequality and take the properties of the two functions involved into account. The limitation in Eq. (13) implies that \( w_{X''X'}(\eta) \) is absolutely integrable in \( \eta \) and, for the properties of the Fourier transform already used, the off diagonal matrix elements starting from the initial entangled state \( \rho_{X''X'}^{(sc)} \) tend to zero for \( z \to \pm \infty \), i.e. in the two time directions.

Lastly we will consider the harmonic coupling

\[ W^{(hc)} = -1/2k \sum_i (X - x_i)^2 = -1/2knX^2 + kX \sum x_i - 1/2 \sum x_i^2. \]

The last term is absorbed in \( V(x_1, x_2, \ldots) \), the first only contributes a phase factor to the matrix elements \( \rho_{X''X'}^{(hc)} \) and the rest is the linear coupling we have already seen. Starting from the same initial conditions as in the case of \( W^{(sc)} \), we obtain

\[ \rho_{X''X'}^{(hc)} = \rho_{X''X'}^{(sc)} e^{-ikn(X''^2 - X'^2)t/[2\hbar]}. \] \hspace{1cm} (14)

For the sake of completeness we also consider the analogous quadratic coupling:

\[ W^{(mhc)} = -1/2\mu \sum_i (P - \nu x_i)^2 = -1/(2\mu)nP^2 + \gamma P \sum x_i - \gamma \nu/2 \sum x_i^2. \]

with \( \gamma = \nu/\mu \). Here too the last term is absorbed in the potential part of the environment hamiltonian, the first only contributes a phase factor and the rest is just the coupling \( W^{(mc)} \). Starting from the initial (factorized) state considered in that case:

\[ \rho_{P''P'}^{(mhc)} = \rho_{P''P'}^{(mc)} e^{-in(P'^2 - P''^2)t/[2\mu\hbar]}. \] \hspace{1cm} (15)

4. CONCLUDING REMARKS
The most significant result obtained using this environment model, in the limit of infinite mass for the macroscopic body, has been to show that decoherence occurs on the position basis in the case of linear coupling $W^{(sc)}$ and harmonic coupling under very general initial conditions. We have only proven that decoherence occurs as time is going towards infinity, and we cannot therefore exclude the hypothesis that the spatial correlations of body $B$ may increase during finite periods. However, when the initial state was factorized we saw that the absolute values of the off diagonal elements of the reduced density matrix not only go asymptotically to zero but also can never exceed their initial value. That particular initial condition so look as preferred with respect this point. In the case of this type of initial condition we have also showed the time dependency with which the matrix elements in question go asymptotically to zero. The speed at which they do so depends on the initial state of the environment.

In the case of coupling $W^{(sc)}$ we defined a time scale $\tau^{(sc)} = \hbar/[nk(X' - X'')\Delta \eta]$, where $\Delta \eta$ is the initial distribution width of the environment’s centre of mass position. We may assume that decoherence is established when $|t| \gg \tau^{(sc)}$. We have not attempted a quantitative estimate of $\tau^{(sc)}$ as our model is far from realistic. Qualitatively, however, we observed that as well as depending on the environment through the initial mean square deviation of $\eta$, it is inversely proportional to the difference $X' - X''$, to the strength of coupling constant and to the number of particles $n$ with which the macroscopic body interacts. This sort of dependence is certainly reasonable and in passing we note that decoherence occurs, of course after a greater time interval, even with very small coupling constants and through interaction with a single particle. It follows that the influence of the environment on the quantum state of a macroscopic body cannot be ignored and has dramatic effects, however weak.

Still in the case of a factorized initial state, we saw how the preferred basis (i.e. on which the macroscopic body’s reduced density matrix becomes diagonal) depends on the type of interaction with the environment. It is the position basis in the case of linear $W^{(sc)}$ and harmonic coupling and the momentum basis in the case of $W^{(mc)}$ coupling. The preferred basis in our case is the one of the operator commuting with the interaction Hamiltonian. The importance of an interaction commuting with the preferred basis was first stressed by Zurek[21]. Our results so provide further confirmation of what is generally taken for granted, i.e. that the natural preferred basis for
a macroscopic body is the position basis, because the system interacts with the rest of the world through spatial co-ordinates.

Another point to note is that our results are independent of whether or not there is an interaction potential between the particles making up the environment. This means, in our example at least, that decoherence need not be thought of as linked to a thermalization process. On the other hand, this could also be inferred from the case of decoherence due to scattering and, in fact, our model describe a scattering by independent particles when there is no interaction between them.

To conclude we note that in the present model, which assume the whole system of macroscopic body plus the environment as a closed system, decoherence is not an irreversible process. This is made clear in our study by following the evolution of the pure state of the whole system, and because the results obtained are asymptotically valid in the two time directions. The situation would be quite different for a more realistic permanent flux of incoming particles without initial correlation. But our model allows for processes with suitable initial conditions (though difficult to realize in practice and which in our case cannot be factorized) for which the spatial correlations of the macroscopic body increase over a finite time. None of this prevents decoherence from occurring asymptotically. In my opinion this situation calls to mind the spread of the wave packet of a free particle. Depending on the initial conditions it may even contract at the outset, but it will always end up expanding asymptotically.

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