Decoherence : An Irreversible Process

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Abstract

A wide-ranging theory of decoherence is derived from the quantum theory of irreversible processes, with specific results having for their main limitation the assumption of an exact pointer basis.

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Decoherence has become widely recognized as an essential step for understanding and interpreting quantum mechanics. It has been mainly investigated on solvable models, which give most of what we know about the effect; but though some of these models are considered as realistic in a definite situation (for instance in quantum optics [1]), they remain in most cases rather far from reality. Now that the importance of decoherence is acknowledged, it certainly requires a wider theory, and forthcoming investigations will also need more precise results (particularly in the research on quantum computers, where decoherence is expected to be the main obstacle and must be controlled quantitatively).

A simple starting point for such a theory consists in noting that decoherence is an irreversible process, so that one can apply the rather general theories for such processes. It is generally agreed that the best theories of that sort rely on the so-called “projection method” [2–5]. There have already been some attempts to apply it to decoherence [6], but the results in the present Letter improve on them on at least three significant points:

1. One can always define an average part in the coupling of the system with the environment, and when that part is removed the remaining coupling consists only of fluctuations; one can therefore extend considerably the range of perturbation theory.

2. A rather general master equation for decoherence is obtained (Eq. (12) below).

3. Precise quantitative equations are obtained for decoherence, at least when an exact “pointer basis” exists [7].

As far as the overall framework is concerned, one assumes as usual that the system under consideration can be split into a “collective” subsystem with hamiltonian $H_c$ and an environment having a very large number of degrees of freedom with hamiltonian $H_e$. The two systems are coupled, and the full hamiltonian is $H = H_c \otimes I_e + I_c \otimes H_e + H_1$, the coupling $H_1$ allowing energy exchanges and other mutual influences (including decoherence) between the collective system and the environment. The full density operator $\rho$ evolves according to the basic equation
\[ \dot{\rho} = -i[H, \rho] \quad . \] (1)

The main features of the projection method for a typical irreversible process are as follows. A (countable or not) set of independent “relevant observables” \( A^i \) (including the identity \( I \)) is selected. Their “exact” average values, resulting from the exact density operator \( \rho(t) \), are denoted by \( a^i(t) \). A time-dependent test density operator \( \rho_0(t) \) is then introduced with the assumptions (i) that it gives the exact average values \( \{a^i(t)\} \) for the relevant operators \( \{A^i\} \) (so that one might know them if \( \rho_0 \) is known), and (ii) that its information content is minimal. It must be of the form

\[ \rho_0 = \exp \left( -\lambda_i A^i \right) \quad , \] (2)

with Lagrange parameters \( \lambda_i \); summation over repeated indices is assumed as usual, and \( \rho_0 \) is normalized since the identity \( I \) belongs to the set of relevant observables. Auxiliary “densities” (or more properly trace-class operators) are then defined by \( s_i = \partial \rho_0 / \partial a^i \). They satisfy the orthogonality properties,

\[ \text{Tr} \left( s_i A^j \right) = \delta^j_i \quad , \] (3)

which amount essentially to \( \partial a^j / \partial a^i = \delta^j_i \).

The theory makes use of “superoperators”, acting linearly on a trace-class operator to yield a similar operator. For instance, Eq. (1) can be written conventionally as \( \dot{\rho} = \mathcal{L} \rho \), where \( \mathcal{L} \) is the so-called Liouville superoperator. Another superoperator is defined in the projection approach by

\[ \mathcal{P} = s_i \otimes A^i \quad , \] (4)

which means that \( \mathcal{P} \) acts on a trace-class operator \( \mu \) to give \( \mathcal{P} \mu = \text{Tr}(A^i \mu)s_i \). Eq. (3) implies the projection property \( \mathcal{P}^2 = \mathcal{P} \). A relevant density operator is defined as \( \rho_1 = \mathcal{P} \rho \). It also yields the exact quantities \( \{a^i\} \) as average values of the relevant operators \( \{A^i\} \), in view of Eq. (3). Denoting by \( \mathcal{J} \) the identity superoperator, one also introduces the superoperator \( \mathcal{Q} = \mathcal{J} - \mathcal{P} \) which satisfies the same projection properties.
Denoting $Q \rho$ by $\rho_2$ (so that $\rho = \rho_1 + \rho_2$), and applying $P$ and $Q$ to both sides of Eq. (1) one obtains evolution equations for $\rho_1$ and $\rho_2$:

$$\dot{\rho}_1 = P L P \rho_1 + \dot{P} P \rho_1 + P L Q \rho_2 + \dot{P} Q \rho_2,$$

$$\dot{\rho}_2 = Q L Q \rho_2 - \dot{Q} Q \rho_2 + Q L P \rho_1 - \dot{Q} P \rho_1.$$  

When applying the projection method to decoherence, it will be convenient to introduce a commuting set of collective observables $X$ whose eigenvalues $x$ are either discrete or continuous. The “relevant observables” $\{A^i\}$ are chosen to consist of the identity $I$, the environment Hamiltonian $I_e \otimes H_e$ and the collective observables $(|x \geq \pm |x'\rangle \cdot (|x| \pm \pm x| \cdot (|x| \pm i |x'| \otimes I_e$ for every pair $(x, x')$ of eigenvalues of $X$. One can use more simply the set of non-hermitian operators $A^{xx'} = |x \geq x'| \otimes I_e$, which clearly provide a basis for the collective observable. The test density operator (2) takes then the simple form

$$\rho_0 = \rho_c \otimes \rho_e,$$

where $\rho_c$ turns out to be the familiar reduced density operator for the collective subsystem and $\rho_e$ is, at least formally, a normalized density operator for the environment as if it were in thermal equilibrium:

$$\rho_c = \text{tr} \rho, \quad \rho_e = \exp (-\alpha - \beta H_e).$$

Throughout I denote a partial trace over the environment by $\text{tr}$ and a full trace by $\text{Tr}$. The time-depending parameters $\alpha$ and $\beta$ are chosen so that $\rho_e$ is normalized and the “exact” average value $E$ for the environment energy is obtained from it. It should be stressed that this expression of $\rho_e$ does not mean that the environment is in thermal equilibrium; it means only that one does not need to know more than the average environment energy in order to obtain collective quantities, including the reduced density operator.

The first part of the calculation consists in obtaining algebraically obtaining the auxiliary densities $s_i$, which are given here for convenience (using the notation $s(A^i)$ in place of $s_i$).
\[ s(|x><x'| \otimes I_e) = |x'><x'| \otimes \rho_e , \]
\[ s(I_c \otimes H_e) = I_c \otimes (\rho_e (H_e - E)) \Delta^{-2} ; \quad s(I) = -E I_c \otimes (\rho_e (H_e - E)) \Delta^{-2} \]

with \( \Delta^2 = tr(H_e^2 \rho_e) - E^2 \), so that acting on a trace-class operator \( \mu \), the projection superoperator \( \mathcal{P} \) gives

\[ \mathcal{P} \mu = (tr \mu) \otimes \rho_e + I_c \otimes (\rho_e (H_e - E)) \Delta^{-2} \{ Tr (H_e \mu) - E Tr \mu \} . \quad (9) \]

(In particular, \( \rho_1 = \rho_0 \)).

Then comes an important trick. It is very convenient to introduce an average collective coupling

\[ \Delta H_c = tr (H_1 \cdot I_c \otimes \rho_e) , \]

which is a collective operator representing a collective effect of the environment (for instance the action of pressure in the case of a gaseous environment). It is generally important, though equal to zero in a few special cases (matter-radiation coupling, nuclear magnetic resonance, and some oscillator models). The remaining part of the coupling \( H'_1 = H_1 - \Delta H_c \otimes I_e \), consists presumably in most cases of small fluctuations, which can be considered as perturbations of the hamiltonian \( H_0 = (H_c + \Delta H_c) \otimes I_e + I_c \otimes H_e \). To second order in \( H'_1 \), Eqs. (5-6) become explicitly

\[ \dot{\rho}_c = -i[H_c, \rho_c] - i tr[H_1, \rho_2] , \quad (10) \]
\[ \dot{\rho}_2 = -i[H_0, \rho_2] - i[H_1, \rho_0] + i tr[H_0, \rho_2] \otimes \rho_e . \quad (11) \]

One can solve Eq. (11) for \( \rho_2 \) as a function of \( \rho_0 \), using first-order perturbation theory and assuming for convenience that the environment is in thermal equilibrium at an initial time \( t = 0 \) so that \( \rho_2(0) = 0 \). Inserting the resulting expression for \( \rho_2 \) into Eq. (10), one obtains the rather simple and fundamental “master equation”

\[ \dot{\rho}_c = -i[H_c + \Delta H_c, \rho_c] - \int_0^t dt' tr \left\{ [H'_1, U[H'_1, \rho_0(t')]U^{-1}] \right\} , \quad (12) \]
where $U = \exp(-iH_0(t - t'))$.

Though already known when the full coupling $H_1$ is weak, Eq. (12) has a much wider range of valid since it holds for a fluctuating $H'_1$. The last step in the calculation consists in writing down explicitly the master equation, explicit expressions being obtained when the basis $|x>$ is an exact pointer basis or, more precisely, when $H'_1$ and $X$ commute so that $H'_1$ is diagonal in the $|x>$ basis and behaves like an operator $V(X)$ in the environment Hilbert space (more explicitly, introducing eigenvectors $|k>$ of $H_e$ with eigenvalues $E_k$, one has $<x,k|x',n> = \delta(x-x')V_k(x)$). The existence of a pointer basis will be assumed from here on.

One can then define a microscopic distance (abbreviated by $\mu D$) between two points $x$ and $x'$ as a distance $|x - x'|$ where the (quantum) first term in the right-hand side of Eq. (12) dominates the value of $\dot{\rho}_c(x,x')$. A small macroscopic distance ($SMD$) will be one for which the second (decoherence) term in the right-hand side dominates, although $x - x'$ is still macroscopically small. I will assume furthermore that $V(x) - V(x')$ depends linearly locally on $x - x'$ with a “slope” $V'$ over small distances ($\mu D$ and $SMD$), which are the only distances of interest in applications. The second (decoherence) term in the right-hand side of the master equation (12) becomes then, for $\mu D$'s and $SMD$'s,

$$-\int_0^t dt' \int dx_1 dx'_1 K(x,x';x_1,x'_1;t-t')\rho_c(x_1,x'_1,t')$$

where the kernel is

$$K = \sum_{n,k,N,M} (x-x') \left[ (x_1-x'_1) \cosh \beta\omega_{kn}/2 + (x_1+x'_1-x-x') \sinh \beta\omega_{kn}/2 \right]$$

$$\times <x'|N><N|x_1><x'_1|M><M|x'> \exp(i\Omega_{MN}\tau)$$

$$\times |V'_{kn}|^2 \exp(-i\omega_{kn}\tau)\bar{\rho}_{nk}.$$  

(14)

By $|N>$, $|M>$, one denotes eigenvectors of $H_e + \Delta H_c$ with eigenvalues $E_N$, $E_M$, and $\Omega_{MN} = E_M - E_N$, similarly $\omega_{kn} = E_k - E_n$ and $\bar{\rho}_{nk} = \exp[-\alpha - \beta(E_k + E_n)/2]$, and $\tau = t - t'$.

This expression has many interesting consequences:
1. The results of previous models can be recovered, often resulting in a simpler kernel; for instance, models with an environment consisting of a collection of two-states systems (one system for each $\omega$), or harmonic oscillators. Decoherence by collisions with an environment of molecules or photons is best obtained by using plane-wave states for $n$ and outgoing scattering states for $k$.

2. Both terms involving $\cosh \beta \omega/2$ and $\sinh \beta \omega/2$ in Eq. (14) are significant at low temperature and $\mu D$’s. This case will be presumably important for future technology when decoherence and quantum coherence compete.

3. The interpretation of quantum measurements, with suppression of macroscopic superpositions (as in the Schrödinger cat problem), is mainly concerned with macroscopic values of $(x - x')$, or $SMD$’s. One can then put $x_1 = x$ and $x'_1 = x_1$, as can be shown easily when $H_c = P^2/2m$ by means of Fourier transforms. The case $H_c = P^2/2m + W(x)$ requires a more elaborate justification using coherent collective states or microlocal analysis, but one always obtains for $SMD$’s

$$ K \simeq \sum_{n,k} \delta(x - x_1)\delta(x' - x'_1)(x - x')^2 \cosh(\beta \omega_{kn}/2)$$
$$ \times |V'_{kn}|^2 \exp[-i\omega_{kn}(t - t')] \bar{\rho}_{nk} \quad (15) $$

4. At high enough temperature and when retardation in $t - t'$ is neglected, the decoherence term at $SMD$’s becomes simply $-\mu(x - x')^2$, with a decoherence coefficient

$$ \mu \simeq -\sum_{n,k} |V'_{kn}|^2 (\omega_{kn} - i0)^{-1} \bar{\rho}_{nk} \simeq \pi \sum_{n,k} |V'_{kn}|^2 \bar{\rho}_{nk} \delta(\omega_{kn}) \quad (16) $$

5. If $P$ is the momentum canonically conjugate to $X$, one finds easily that the term in $\cosh \beta \omega/2$ in Eq. (14) does not contribute to $< dP/dt >$, i.e. to damping. The term in $\sinh \beta \omega/2$ gives on the other hand gives a damping

$$ < dP/dt > = \text{forces} - \int_0^t D(t - t') < P(t') > dt' \quad , \quad (17) $$
with
\[ D(\tau) = 2m^{-1} \sum_{n,k} |V'_{kn}|^2 \bar{\rho}_{nk} e^{-i\omega \tau} \sinh(\beta \omega_{kn}/2) \omega_{kn}^{-1} . \]

This simple result results from several steps: The action of \( P = -i\partial/\partial x \) on the kernel \( K \) (in Eq. (14)) removes the factor \( (x - x') \) since other terms in the derivative containing this factor have zero average. The integral over \( x \) of \( < x|N > < M|x > \) gives simply \( \delta_{NM} \). A term such as \( x < x|N > < M|x > \exp(i\Omega \tau) \) is expressed as \( < M|U_c^+ X U_c|N > \), with \( U_c = \exp(-iH_c\tau) \). One can then use the equation

\[ [X, U] = UP\tau/m , \quad (18) \]

which is exact for \( H_c = P^2/2m \) and valid up to higher orders in \( \hbar \) in the presence of a collective potential. The factor \( \tau \) in Eq. (18) is finally removed by integrating by parts on \( \tau \). Other more direct methods also exist for evaluating damping, and they agree with the result.

When retardation effects are again neglected, the damping term in Eq. (17) becomes \( -\gamma < P > \) and, at high enough temperature, one recovers the well-known relation \( \mu = mkT\hbar^{-2} \), where Planck’s constant has been reintroduced. One might also derive the familiar expression \( -\gamma/2(x - x')(\partial/\partial x - \partial/\partial x')\rho_c(x, x') \) for damping with similar approximations.

To conclude, the main limitation of the final results following Eq. (12), is the assumption of an exact pointer basis. Such bases are known to exist for a strictly mechanical collective system (the \( X \)’s being the position coordinates of coarse-grained pieces of matter in the macroscopic system), or in the case of SQUID loops [7]. More generally, approximate diagonalization occurs also presumably in a basis of coherent states [11] although the validity of the present analysis remains uncertain in that case, as well as its relation with classical behavior [12].

Finally, the increase of entropy resulting from irreversibility is mainly found in the increase of \( -Tr(\rho_c \text{ Log } \rho_c) \) when \( \rho_c \) becomes approximately diagonal.

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Footnotes and References

(a) Eq. (12) was first obtained as a consequence of a guess with *a posteriori* justification [7]. In the same paper, I also attempted its derivation by the projection method, although making unfortunately a few self-compensating errors. No applications except trivial ones were given.

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