Decoherence, Purification and Entanglement

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Abstract

A pure quantum state is a projection on into linear space of quantum mechanics. But this may become, through a quantum stochastic map, a convex sum of projections (and hence an impure state) by decoherence. This is not a superposition. To get superposition we need to restore phase relations and that involves a fiducial projector. As this projector varies the various possible coherent combinations of the components of the mixture may be obtained. By a further application of this method the quantum entanglement between two subsystems can be restored. These methods can be used to maintain long term phase relations by the state being repeatedly processed by purification with possible applications to storage and processing information in quantum computing. In particular from separable or partially separable states we can obtain a purely entangled state.

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I. PURE AND IMPURE STATES: DENSITY MATRICES AND MAPPINGS

There are two ways of specifying a (pure) state of a quantum system. The first version associates with every quantum state a vector of unit norm in a complex inner-product space [1]. This is an overcomplete representation since the (absolute) phase of the state vector is irrelevant; we are in fact dealing with ‘rays’. But if we have to superpose two pure states to form a pure state, the relative phase of the two state vectors is relevant (but their absolute phases are not). This method of representing states by vectors has another shortcoming in that it cannot represent mixed states. These can only be represented by assigning probabilities to a collection of states and averaging over all relative phases.

To surmount these shortcomings another method is to associate a pure state with projections in the complex inner product space [2]. There is no redundant phase. The impure states are formed by convex combinations of such projections. These states correspond to a normalized nonnegative linear operator called the density matrix rather than to rays. Any mechanism of corrupting the relative phases in a superposition is a process of ‘decoherence’. The decoherence phenomenon of pure states into mixtures can be easily treated in terms of density matrices by looking at it as an instance of a broader class of linear maps acting on a pure density matrix. Such linear maps of density matrices has been studied under the title of (convex) stochastic maps and will be discussed in section IV.

Given a coherent superposition we can decohere it partly or totally to get an impure state density matrix. We may raise the reverse problem: given a mixed state, can we restore the relative phase? In particular, can we make a pure state but with the same probabilities?

II. PURIFICATION

It is remarkable that this can be done by a simple protocol called ‘purification’ originally pointed out by Schrodinger. [7]. We first illustrate it in the mixture of two orthogonal states:

$$\rho' = p_1 \rho_1 + p_2 \rho_2$$

$$\rho_1^2 = \rho_1 , \rho_2^2 = \rho_2 , \text{tr}(\rho_1 \rho_2) = 0 , \text{tr}(\rho_1) = \text{tr}(\rho_2) = 1.$$
Now we use the construction [6]

$$\rho = p_1 \rho_1 + p_2 \rho_2 + \frac{\rho_1 \Pi \rho_2}{\sqrt{\text{tr}(\rho_1 \Pi) \text{tr}(\rho_2 \Pi)}}. \quad (1)$$

It is easily verified that this is a pure state. $\Pi$ is a projection which is not orthogonal to $\rho_1$ or $\rho_2$. As $\Pi$ varies so does $\rho$, and the relative phase depends on the choice of $\Pi$. We can show that any desired phase can be so obtained.

For a mixture of more than two projections we need only to generalize the formula above:

$$\rho = \sum_{i,j} \sqrt{p_i p_j} \frac{\rho_i \Pi_j \rho_j}{\sqrt{\text{tr}(\rho_i \Pi) \text{tr}(\rho_j \Pi)}}. \quad (2)$$

We shall extend the purification of a separable density matrix of a bipartite system to restore full quantum entanglement.

III. STOCHASTIC MAPS FROM HAMILTONIAN SYSTEMS

Now that we have seen that there exists a simple way of restoring the coherence in a mixed state we can take a closer look at the process of decoherence itself. First let us consider how from a Hamiltonian system we could derive (irreversible) stochastic maps. For clarity we start with a two-level system with states $|1\rangle$ and $|2\rangle$ and a time-independent Hamiltonian

$$H = g(|1\rangle\langle 2| + |2\rangle\langle 1|) + \frac{\nu}{2}(|1\rangle\langle 1| - |2\rangle\langle 2|). \quad (3)$$

If we choose the term proportional to $\nu$ as the interaction part of the Hamiltonian, then in the interaction picture the Hamiltonian becomes time dependent

$$H_I = g(e^{i\nu t}|1\rangle\langle 2| - e^{-i\nu t}|2\rangle\langle 1|). \quad (4)$$

Under this ‘perturbation’, the states $|1\rangle$ and $|2\rangle$ are no longer stationary but undergo Rabi oscillations. There is no decoherence. But if we take times small compared with $\nu^{-1}$ and compute only the probabilities for the states $|1\rangle$ and $|2\rangle$, we find a decoherent evolution. When we generalize this to a system with many frequencies which are small integral multiples of a single frequency, we get a collection of partial revivals reminiscent of Talbot’s bands in optics. The problem of the time dependence of an arbitrary state of a free particle was studied by W. Schleich and collaborators (called a “quantum carpet”) [9] The relative phases endure naturally, and they are essential in the buildup of the Talbot resonances.
Qualitatively new features obtain when a discrete energy state is coupled to a continuum of energies. This is the model studied by Dirac [1] (which has had reincarnations as Friedrich’s model, the Lee model and the Jaynes-Cummings model) to formulate the semi-classical theory of radiative de-excitation of an excited state of an atom. The amplitude for transition from the discrete state to the continuum is

\[ h(\alpha'', \alpha') = \langle \alpha'' | V^* (t') | \alpha' \rangle = \langle \alpha'' | V | \alpha' \rangle e^{i(E'' - E') t'} , \]  

where \( |\alpha''\rangle \) is the discrete state and \( |\alpha'\rangle \) is a state belonging to the continuum. If we wait for a small time \( t \) the amplitude for transition is

\[ \int_0^t dt' \langle \alpha'' | V^* (t') | \alpha' \rangle = \langle \alpha'' | V | \alpha' \rangle \frac{e^{i(E'' - E') t} - 1}{t(E'' - E')} . \]  

The discrete state at \( t = 0 \) becomes a superposition (not a mixture) of the continuum states.

\[ |\alpha''\rangle \rightarrow \left( \sqrt{1 - \int |h(\alpha'', \alpha')|^2 dE'} \right) |\alpha''\rangle + \int h(\alpha'', \alpha') e^{-iE't} |\alpha'\rangle . \]  

This state is a pure state whether \( t \) is positive or negative. This transformation is unitary and reversible. If, following Dirac, we ask for the probability of a state with continuum energy and we have the probability density

\[ \rho(\alpha'', \alpha') \, d\alpha' = |h(\alpha'', \alpha')|^2 \, d\alpha' . \]  

By integrating over the frequency and making some approximation appropriate for not too small a time, he deduces a decay probability proportional to time \( t \) (with \( t > 0 \)). So we see that the irreversible process is due to decoherence that is introduced when we look at the probabilities (with the relative phases being lost) rather than due to the interaction itself!

This conclusion is dramatically demonstrated if we start with a continuum superposition for \( t = - |t'| \). In other words we take as our intial state corresponding to \( t = 0 \), that state which is obtained by evolving the original discrete state backwards in time for \( |t'| \) seconds. Such a state would recombine to become the excited discrete state precisely when \( t = |t'| \).

This remark about the relative phases and the role of decoherence in some (apparently irreversible) processes is seen in the time development of a free particle with an initial state minimum uncertainty wave function

\[ \psi (x) = \pi^{-\frac{1}{4}} e^{-x^2/2} \]  

\[ \langle x^2 \rangle = \frac{1}{2} . \]
Then under free particle evolution this Gaussian packet spreads. The new mean square position is

\[ \langle x^2(t) \rangle = \frac{1}{2 \sqrt{1 + (t/m)^2}} = \frac{1}{2} \left[ 1 + \left( \frac{t}{m} \right)^2 \right]^{-1/2} \]

Does this mean that a Gaussian packet always expands? Yes, if the wave function was real at time \( t = 0 \). But if we had a suitable phase \( e^{iHt}\psi(x, 0) \), then the mean square position variable will shrink from \( t = 0 \) to \( t = \tau \) and then start expanding. This may be seen even more clearly if we look at the wave function in the momentum space: the minimum uncertainty state is

\[ \tilde{\psi}(p, 0) = \pi^{-\frac{1}{4}} e^{-p^2/2}. \]

Then it will expand as time goes by since the wave function at time is

\[ \tilde{\psi}(p, t) = e^{-i p^2t/2m} e^{-p^2/2}. \]

So the wave function at an earlier time \( t = -\tau \) would have been

\[ \tilde{\psi}(p, -\tau) = e^{i p^2\tau/2m} e^{-p^2/2}. \]

This wave function contracts as time increases from \( -\tau \) to 0 and then expands.

**IV. DECOHERENT EVOLUTIONS: EXTREMAL MAPS**

The decoherent evolution of a quantum system leads to a stochastic map which is a contraction of the convex set of density matrices which converge to one (or more) fixed density matrices. In contrast, a unitary (reversible) evolution yields a map which takes the density matrices on to themselves, in particular a pure density matrix. The trace orthogonality of two density matrices \( \rho_1 \) and \( \rho_2 \) would not be preserved by a stochastic map

\[ \text{tr}(\rho'_1 \rho'_2) \neq \text{tr}(\rho_1 \rho_2), \]

while the unitary evolutions preserve the trace orthogonality

\[ \text{tr}(\rho_1 \rho_2) = 0 \implies \text{tr}(\rho'_1 \rho'_2) = 0, \]

The stochastic maps themselves constitute a convex set [3]. It would be of interest to construct the extremal set of such dynamical maps. The maps themselves satisfy the following
properties (repeated indices are summed over).

\[ \rho_{rs} \rightarrow B_{rr', ss'} \rho_{rr'} > 0, \]  

so that

\[ x_ry^*_r B_{rr', ss'} x_s y^*_s > 0, \]  

\[ \sum B_{rr', ss'} = \delta_{r', s'}, \]

and may be parametrized in terms of the eigenvectors of \( B \) in the form

\[ B_{rr', ss'} = \mu(\alpha)C_{rr'}(\alpha)C^\dagger_{ss'}(\alpha), \]

where \( \mu(\alpha) \) may be positive or negative. If all the \( \mu(\alpha) \) are positive, the map is said to be “completely positive” [4]. In this case the positive eigenvalue \( \mu(\alpha) \) may be absorbed into the eigenmatrix \( C(\alpha) \) so that a completely positive map may be described by a number \( R \leq N \) matrices in the form

\[ \rho' = \sum_{a=1}^{\mathcal{R}} C_a \rho C^\dagger_a, \quad \sum_{a=1}^{\mathcal{R}} C^\dagger_a C_a = 1. \]  

If we take the system \( S \) with density matrix \( \rho_{rs} \) to be coupled to an external ‘reservoir’ system \( R \) in the form

\[ \rho_{rs} = \sum a R_{ar, as}, \]

then the evolution is by stochastic maps which are completely positive. The reservoir system is not unique, nor is the coupling between the concerned system and the reservoir.

We may write down the completely positive map as the contraction of a unitary map of an extended system as follows;

\[ \rho_{jk} \rightarrow V_{n_{j'k'}} \rho_{jk} \tau_{d'b'} V^\dagger_{d'b', nk}, \]

with

\[ V^\dagger_{a_{j'k'}} V_{a_{j'k'}, b_{k'}} = \delta_{ab} \delta_{jk}; \quad \tau_{aa} = 1. \]  

Such a map is completely positive. It will be extremal if \( \tau \) is a projection

\[ \tau ac \tau cb = \tau ab. \]  

The inverse construction also can be carried out to embed any stochastic map (which is completely positive) as the unitary evolution of the larger system [5]. Extremal maps corresponds to projection valued \( \tau_{ab} \).
It would be illustrative to construct all extremal maps of rank $R \leq 3$ for a $3 \times 3$ system:
if $R = 1$, the condition

\[ C^\dagger C = 1 , \]
implies that the map is unitary. (Antiunitary maps are not completely positive.) The first nontrivial case is for $R = 2$. In this case we have

\[ \rho \rightarrow C^\dagger (1) \rho C(1) + C^\dagger (2) \rho C(2) \]

\[ C(1) C^\dagger (1) + C(2) C^\dagger (2) = 1 . \]

We can always find unitary matrices $U,V$ such that

\[ C(1) = U^\dagger D(1) V , \]

where $D(1)$ is a nonnegative diagonal matrix.

\[ D^2(1) = U C(1) C^\dagger (1) U^\dagger = U [1 - C(2) C^\dagger (2)] U^\dagger = 1 - D^2(2) . \]

We may choose

\[
D(1) = \begin{pmatrix}
\cos \theta_1 & 0 & 0 \\
0 & \cos \theta_2 & 0 \\
0 & 0 & \cos \theta_3 
\end{pmatrix}
\]

\[
D(2) = \begin{pmatrix}
\sin \theta_1 & 0 & 0 \\
0 & \sin \theta_2 & 0 \\
0 & 0 & \sin \theta_3 
\end{pmatrix}
\]

Then

\[ C(2) = U^\dagger D(2) W \]

where $W$ is an arbitrary unitary matrix. The generic map of rank 2 is

\[ \rho \rightarrow V^\dagger D(1) U \rho U^\dagger D(1) V + W^\dagger D(2) U \rho U^\dagger D(2) W . \]

For rank 3 ($R = 3$), the construction is as follows:

\[ C(1) = U^\dagger D(1) V \]

\[ C(2) C^\dagger (2) + C(3) C^\dagger (3) = 1 - U^\dagger D^2(1) U . \]
If $D(1)$ is chosen as

$$D(1) = \begin{pmatrix}
\cos \theta_1 & 0 & 0 \\
0 & \cos \theta_2 & 0 \\
0 & 0 & \cos \theta_3
\end{pmatrix}$$

then

$$C(2) C^\dagger(2) + C(3) C^\dagger(3) = U^\dagger \begin{pmatrix}
\sin^2 \theta_1 & 0 & 0 \\
0 & \sin^2 \theta_2 & 0 \\
0 & 0 & \sin^2 \theta_3
\end{pmatrix} U.$$

We may write

$$C(2) = U^\dagger \begin{pmatrix}
\sin \theta_1 & 0 & 0 \\
0 & \sin \theta_2 & 0 \\
0 & 0 & \sin \theta_3
\end{pmatrix} V \begin{pmatrix}
\cos \phi_1 & 0 & 0 \\
0 & \cos \phi_2 & 0 \\
0 & 0 & \cos \phi_3
\end{pmatrix} W,$$

$$C(3) = U^\dagger \begin{pmatrix}
\sin \theta_1 & 0 & 0 \\
0 & \sin \theta_2 & 0 \\
0 & 0 & \sin \theta_3
\end{pmatrix} V \begin{pmatrix}
\sin \phi_1 & 0 & 0 \\
0 & \sin \phi_2 & 0 \\
0 & 0 & \sin \phi_3
\end{pmatrix} X,$$

where $V, W$ and $X$ are unitary matrices. Verify that

$$C(2) C^\dagger(2) + C(3) C^\dagger(3) = U^\dagger \begin{pmatrix}
\sin^2 \theta_1 \cos^2 \phi_1 & 0 & 0 \\
0 & \sin^2 \theta_2 \cos^2 \phi_2 & 0 \\
0 & 0 & \sin^2 \theta_3 \cos^2 \phi_3
\end{pmatrix} U + U^\dagger \begin{pmatrix}
\sin^2 \theta_1 \sin^2 \phi_1 & 0 & 0 \\
0 & \sin^2 \theta_2 \sin^2 \phi_2 & 0 \\
0 & 0 & \sin^2 \theta_3 \sin^2 \phi_3
\end{pmatrix} U$$

$$= U^\dagger \begin{pmatrix}
\sin^2 \theta_1 & 0 & 0 \\
0 & \sin^2 \theta_2 & 0 \\
0 & 0 & \sin^2 \theta_3
\end{pmatrix} U.$$

Hence

$$C(1) C^\dagger(1) + C(2) C^\dagger(2) + C(3) C^\dagger(3) = 1.$$

The map is

$$\rho \rightarrow X^\dagger \begin{pmatrix}
\sin \phi_1 & 0 & 0 \\
0 & \sin \phi_2 & 0 \\
0 & 0 & \sin \phi_3
\end{pmatrix} V^\dagger \begin{pmatrix}
\sin \theta_1 & 0 & 0 \\
0 & \sin \theta_2 & 0 \\
0 & 0 & \sin \theta_3
\end{pmatrix} U \rho.$$
\[ \times U^\dagger \begin{pmatrix} \sin \theta_1 & 0 & 0 \\ 0 & \sin \theta_2 & 0 \\ 0 & 0 & \sin \theta_3 \end{pmatrix} V \begin{pmatrix} \sin \phi_1 & 0 & 0 \\ 0 & \sin \phi_2 & 0 \\ 0 & 0 & \sin \phi_3 \end{pmatrix} X + W^\dagger \begin{pmatrix} \cos \phi_1 & 0 & 0 \\ 0 & \cos \phi_2 & 0 \\ 0 & 0 & \cos \phi_3 \end{pmatrix} V^\dagger \begin{pmatrix} \sin \theta_1 & 0 & 0 \\ 0 & \cos \theta_2 & 0 \\ 0 & 0 & \cos \theta_3 \end{pmatrix} U \rho \]

No generality is lost by choosing an orthogonal transformation among \( C(1), C(2), C(3) \) to make
\[ \cos \theta_3 = 1 \quad \cos \phi_3 = 1. \]

Hence the generic map is defined by the \( SU(3)/Z_3 \) matrices \( U, V, W, X \) and the angles \( \theta_1, \theta_2, \phi_1, \phi_2 \).

The indecomposable set \( C(1), C(2), C(3) \) serve to preserve the trace but degrade some of the phases in \( \rho \). The essential irreversibility is thus decoherence induced.

V. **ENTANGLED SYSTEMS, DECOHERENCE AND PURIFICATION**

A closely related quantum property is that of 'quantum entanglement' [7] If we have the density matrix \( R \) of a bipartite system \( AB \), which may or may not be pure, then the partial traces
\[ \text{tr}_B R_{AB} = \rho_A \quad \text{tr}_A R_{AB} = \rho_B \]
do not in general contain all the information in \( R \). If \( R_{AB} \) is a pure state, \( \rho_A \) and \( \rho_B \) need not be pure, but they will have the same eigenvalues. If \( \rho_A \) is pure, so is \( \rho_B \) and \( R_{AB} \) is a direct product.
\[ R_{AB} = \rho_A \otimes \rho_B. \]
So $R_{AB}$ is separable. More generally if

$$R_{AB} = \sum_n p_n \rho_A(n) \otimes \rho_B(n) \ , \ \sum_n p_n = 1 \ , \ p_n \geq 0 , \quad (20)$$

then $R_{AB}$ is said to be separable. But for a generic pure state $R_{AB}$, $\rho_A$ and $\rho_B$ need not be pure. This obtains for example for the ‘singlet’ state

$$\Psi_{AB} = \frac{1}{\sqrt{2}} (\chi_A \varphi_B - \chi_B \varphi_A) ,$$

for which

$$R_{AB} = \Psi_{AB} \Psi_{AB}^\dagger ; \quad \rho_A = \frac{1}{2} (\chi_A \chi_A^\dagger + \varphi_A \varphi_A^\dagger) ;$$

the partial traces are not pure.

Thus the difference between the projection $R_{AB}$ and $\rho_A \otimes \rho_B$ is the averaging over the phases of the interference terms $\chi_A \chi_B^\dagger$ and $\chi_B \chi_A^\dagger$. It follows that to restore the pure state from the separable impure state $\rho_A \otimes \rho_B$ is the restoration of the interference terms. But they are ambiguous since

$$R_{AB}(\theta) = \frac{1}{2} (\chi_A \varphi_B + e^{i \theta} \varphi_A \chi_B) (\chi_A \varphi_B^\dagger + e^{-i \theta} \varphi_A \chi_B^\dagger) \quad (21)$$

is a pure state giving the same marginal density matrices $\rho_A$ and $\rho_B$. This indeterminateness of the relative phase angle was seen in the ‘purification’ of any impure density matrix.

It is not necessary that $\rho_A$ and $\rho_B$ are multiples of the unit matrix. For example

$$R_{AB} = \Psi_{AB} \Psi_{AB}^\dagger$$

$$\Psi_{AB} = (\cos \alpha \chi_A \varphi_B + \sin \alpha e^{i \theta} \chi_B \varphi_A)$$

leads to the partial density matrices

$$\rho_A = \cos^2 \alpha \chi_A \chi_A^\dagger + \sin^2 \alpha \varphi_A \varphi_A^\dagger$$

from which all information about $\theta$ has disappeared. We could generalize this to a more general $\Psi_{AB}$ of the form

$$\Psi_{AB} = (c_1 \chi_1 \varphi_1 + c_2 \chi_2 \varphi_2 + c_3 \chi_3 \varphi_3 + \ldots)$$

$$\chi_j \chi_k = \delta_{jk} = \varphi_j^\dagger \varphi_k \ ; \ |c_1|^2 + \ldots |c_n|^2 = 1 .$$
The partial trace density matrices are
\[
\rho_A = |c_1|^2 \chi_1 \chi_1^\dagger + |c_2|^2 \chi_2 \chi_2^\dagger + \ldots \\
\rho_B = |c_1|^2 \varphi_1 \varphi_1^\dagger + |c_2|^2 \varphi_2 \varphi_2^\dagger + \ldots .
\]

The purification of either
\[
R\'_{AB} = \rho_A \otimes \rho_B
\]
or
\[
R\''_{AB} = |c_1|^2 \chi_1 \varphi_1 \varphi_1^\dagger + |c_2|^2 \chi_2 \varphi_2 \varphi_2^\dagger + \ldots 
\]
can yield the same set of purified entangled density matrices
\[
R_{AB} = \Psi_{AB} \Psi_{AB}^\dagger
\]
with \( \Psi_{AB} \) as given above, but the relative phases of \( c_1, c_2 \ldots \) completely arbitrary.

The distinction between a ‘simply separable’ density matrix
\[
R_{AB} = \rho_A \otimes \rho_B
\]
and a ‘generic separable’ matrix
\[
S_{AB} = \sum_n p_n \rho_A(n) \otimes \rho_B(n)
\]
is this. The simply separable case has
\[
R_{AB} = \sum_r p(r) \psi(r) \psi^\dagger(r) . . . \phi(r) \phi^\dagger(r) , \sum_r p(r) = 1
\]
with
\[
\psi^\dagger(r) \psi(s) = \delta_{rs} = \phi^\dagger(r) \phi(s) .
\]
But
\[
S_{AB} = \sum_s q(s) \psi(s) \psi^\dagger(s) . . . \phi(s) \phi^\dagger(s) , \sum_s q(s) = 1
\]
has the vectors \( \{ \psi(s) \} \) and \( \{ \phi(s) \} \) not being orthonormal. This decomposition is always possible since
\[
\rho_A(r) \otimes \rho_B(n) = \sum_{n,r} p(n,r) \psi(n,r) \psi^\dagger(n,r) . . . \phi(n,r) \phi^\dagger(n,r)
\]
with
\[
\psi^\dagger(n,r) \psi(n,r') = \delta_{r,r'} = \phi^\dagger(n,r) \phi(n,r')
\]
but no such restriction obtains for

\[ \psi^\dagger(n, r)\psi(n', r'), \phi^\dagger(n, r)\phi(n', r') . \]

Purification in all cases involves the use of a projector \( \Pi \) which has nonzero overlap with any state involved in the decomposition of \( R_{AB} \).

Purification [6] thus leads from a separable system, or any impure system to a pure state which automatically possessed quantum entanglement.

VI. CONCLUDING REMARKS: DECOHERENCE AND IRREVERSIBILITY.

We already saw that the coupling of a discrete state to a continuum does not lead to decay until the relative phases are averaged out. This insight answers an old puzzle: an accelerated charge radiates, but when does the radiation become independent of the accelerated charge? When does the photon really get emitted from the atom? [8] The answer is that when decoherence sets in, the processes have taken place.

But where does this decoherence come from? A finite closed system cannot have irreversible processes. If the system is not finite but is in the thermodynamic limit, no finite subsystem is closed. It is in this limit that we could obtain intrinsic decoherence.

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