A general scheme for ensemble purification

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Abstract

We exhibit a general procedure to purify any given ensemble by identifying an appropriate interaction between the physical system $S$ of the ensemble and the reference system $K$. We show that the interaction can be chosen in such a way to lead to a spatial separation of the pair $S$–$K$. As a consequence, one can use it to prepare at a distance different equivalent ensembles. The argument associates a physically precise procedure to the purely formal and fictitious process usually considered in the literature. We conclude with an illuminating example taken from quantum computational theory.

1 Introduction

A statistical ensemble $\mathcal{E}$ of physical systems $S$ is characterized by a (finite, countable or continuous) set of positive numbers $p_i$ summing up to 1 and by a corresponding set of normalized vectors $|\psi_i\rangle$ of the Hilbert space $\mathcal{H}^S$ associated to the system $S$, so that we will write $\mathcal{E}(p_i, |\psi_i\rangle)$ to represent it. The statistical operator $\rho_\mathcal{E}$ (a trace–class, trace one, semipositive definite operator) associated to $\mathcal{E}(p_i, |\psi_i\rangle)$ is defined as:

$$\rho_\mathcal{E} = \sum_i p_i |\psi_i\rangle \langle \psi_i|.$$  

(1.1)

A point of great conceptual relevance which marks a radical difference between the classical and quantum cases is that, while in classical mechanics the assignment of the statistical operator $\rho(r, p)$ uniquely identifies the ensemble, within quantum mechanics, as it is well known, the correspondence between statistical ensembles and statistical operators is infinitely many to one.

With reference to this point, let us consider the set of all statistical ensembles of systems like the one under consideration. Such a set can be naturally endowed with an equivalence relation.

Definition: We will say that two statistical ensembles $\mathcal{E}$ and $\mathcal{E}^*$ are equivalent, and we will write $\mathcal{E} \equiv \mathcal{E}^*$, iff $\rho_\mathcal{E} = \rho_\mathcal{E}^*$.
It is obvious that the just defined relation is reflexive, symmetric and transitive and that it leads to a decomposition of the set of all ensembles into disjoint equivalence classes. We will denote as $[\mathcal{E}]$ the equivalence class containing the ensemble $\mathcal{E}$.

Purification of an ensemble $[\mathcal{E}]$ is a procedure by which one associates to the ensemble a pure state $|\Psi\rangle$ of an appropriately enlarged Hilbert space $\mathcal{H}^{S+K} = \mathcal{H}^S \otimes \mathcal{H}^K$, where $K$ is a reference system whose Hilbert space $\mathcal{H}^K$ we assume to be infinite-dimensional for reasons which will become clear in a moment.

The fundamental request on $|\Psi\rangle$ is that, by measuring an appropriate observable of $K$ and confining attention to the system $S$ alone, one can prepare the desired ensemble $\mathcal{E}(p_i, |\psi_i\rangle)$.

The first proof that, given two equivalent ensembles $\mathcal{E}(d_i, |\phi_i\rangle)$ and $\mathcal{E}(p_j, |\chi_j\rangle)$, one can find two orthonormal sets $\{|A_i\rangle\}$ and $\{|B_j\rangle\}$ of $\mathcal{H}^K$ such that

$$|\Psi\rangle = \sum_i \sqrt{d_i} |\phi_i\rangle \otimes |A_i\rangle = \sum_j \sqrt{p_j} |\chi_j\rangle \otimes |B_j\rangle$$

(1.2)

has been exhibited by Gisin. This result is particularly relevant since it is related to the request that no faster-than-light signals can be sent between distant observers.

Subsequently, Hughston et al. have generalized the above result, providing a complete classification of equivalent ensembles: using the purification procedure, they have derived necessary and sufficient conditions for two ensembles to be equivalent.

In the literature (see, e.g., [1]), ensemble purification is usually considered as a purely mathematical tool: one does not identify any dynamical mechanism which could be used to actually implement it, and the system $K$ is considered a fictitious system without a direct physical significance. The aim of this paper is to exhibit a precise physical procedure in order to purify any ensemble by making the system $S$ interact with a system $K$, in such a way that the desired pure state $|\Psi\rangle$ be actually produced. Then one can use it to prepare any desired ensemble of the equivalence class.

### 2 Statistical ensembles and the purification process: the constructive procedure

As remarked above, it is our purpose to present a formal constructive mechanism to purify any given ensemble, showing at the same time how, by resorting to this procedure, one can use the obtained pure state to generate all ensembles of systems $S$ equivalent to the one one has purified. The procedure is based on a formalism which parallels strictly the one proposed by von Neumann for implementing ideal measurement processes of the first kind, even though the system $K$, which plays a role analogous to the one of the measuring apparatus in his treatment, can very well be (and actually we will consider it to be) a microsystem.

Our starting point is the consideration of an equivalence class $[\mathcal{E}]$ of ensembles of systems $S$. Within such a class there is the ensemble $\mathcal{E}(d_i, |\phi_i\rangle)$ which corresponds to the spectral decomposition of the associated statistical operator having the positive numbers $d_i$ as eigenvalues and the $|\phi_i\rangle$ as the associated orthonormal eigenvectors. Such a decomposition is unique, apart from accidental degeneracies which, if they occur, can be disposed of as one wants, so that we will consider the eigenvectors $|\phi_i\rangle$ as precisely assigned vectors. We assume that the index $i$ runs from 0 to $n$, without committing ourselves about the fact that $n$ is finite or infinite and about the fact that the orthonormal set $\{|\phi_i\rangle\}$ be a complete set of $\mathcal{H}^S$ or not.
Let us consider now the orthonormal states $|\phi_i\rangle$ and let us assume that there exist a physical system $K$, whose associated Hilbert space $\mathcal{H}^K$ is infinite dimensional, a state $|a_0\rangle$ of $\mathcal{H}^K$ and an interaction hamiltonian $H^{S+K}$ of $\mathcal{H}^{S+K}$ such that the $S$–$K$ interaction lasting for a certain time interval $T$ induces the following evolution:

$$|\phi_i\rangle \otimes |a_0\rangle \rightarrow |\phi_i\rangle \otimes |a_i\rangle, \quad \langle a_i|a_j\rangle = \delta_{ij},$$

(2.1)

where $|a_i\rangle$ are statevectors belonging to $\mathcal{H}^K$.

In the next section we will exhibit a simple hamiltonian having such a property and leading also to an arbitrarily chosen separation in space of the systems $S$ and $K$. We stress that we need $\mathcal{H}^K$ to be infinite dimensional if we want to be able to build a state $|\Psi_T\rangle$ which will allow us to prepare any ensemble whatsoever in the equivalence class under consideration by measurement procedures on systems $K$, since in any equivalence class there are always ensembles containing an infinite number of states.

Given the ensemble $\mathcal{E}(d_i, |\phi_i\rangle)$ we consider the state:

$$|\Psi_0\rangle = \sum_{i=1}^{n} \sqrt{d_i}|\phi_i\rangle \otimes |a_0\rangle,$$

(2.2)

and we let it evolve through the interval $T$. According to Eq. (2.1) and due to the linearity of the quantum evolution, we get

$$|\Psi_0\rangle \rightarrow |\Psi_T\rangle = \sum_{i=1}^{n} \sqrt{d_i}|\phi_i\rangle \otimes |a_i\rangle.$$

(2.3)

We consider now an arbitrary complete orthonormal set $\{|b_j\rangle\}$, $j = 0, 1, \ldots, \infty$, of $\mathcal{H}^K$ and we complete (if necessary) the set $\{|a_i\rangle\}$, $i = 0, 1, \ldots, n$, to a set $\{|A_i\rangle\}$ by adding to it orthonormal states spanning the manifold of $\mathcal{H}^K$ orthogonal to the one generated by the $\{|a_i\rangle\}$ themselves. Obviously we have:

$$|A_i\rangle = \sum_{j=0}^{\infty} U_{ij}|b_j\rangle, \quad i = 0, 1, \ldots, \infty,$$

(2.4)

where $U_{ij}$ is a unitary matrix of $\mathcal{H}^K$. From Eq.(5) we get:

$$|\Psi_T\rangle = \sum_{i=0}^{n} \sum_{j=0}^{\infty} \sqrt{d_i}|\phi_i\rangle \otimes U_{ij}|b_j\rangle$$

$$= \sum_{j=0}^{\infty} \left( \sum_{i=0}^{n} \sqrt{d_i}U_{ij}|\phi_i\rangle \right) \otimes |b_j\rangle$$

$$= \sum_{j=0}^{\infty} |\tilde{\chi}_j\rangle \otimes |b_j\rangle.$$

(2.5)

Note that $\langle \Psi_T|\Psi_T\rangle = 1$ implies:

$$\sum_{j,k=0}^{\infty} \langle \tilde{\chi}_j|\langle b_j|b_k\rangle|\tilde{\chi}_k\rangle = \sum_{j=0}^{\infty} ||\tilde{\chi}_j||^2 = 1.$$

(2.6)

The states $|\tilde{\chi}_j\rangle$ are not normalized, so that, putting $|\chi_j\rangle = |\tilde{\chi}_j\rangle/||\tilde{\chi}_j||$, we have:

$$|\Psi_T\rangle = \sum_{j=0}^{\infty} ||\tilde{\chi}_j|| |\chi_j\rangle \otimes |b_j\rangle.$$

(2.7)

If we measure now an observable of the system $K$ having a non–degenerate spectrum with $|b_j\rangle$ as eigenvectors and we confine our attention to the resulting ensemble of systems $S$, we obtain the ensemble...
\( \mathcal{E}(\| \chi_j \|, \| \chi_j \|) \). Note that since both \( \sum_{i=0}^{n} d_i |\phi_i \rangle \langle \phi_i | \) and \( \sum_{j=0}^{\infty} \| \chi_j \|^{2} |\chi_j \rangle \langle \chi_j | \) are obtained by taking the partial trace on \( \mathcal{H}^{K} \) of \( |\Psi_T \rangle \langle \Psi_T | \), they are equal and the corresponding ensembles belong to the same equivalence class. Thus we have proved that starting from the state \( (2.3) \) and choosing an observable \( E \) to the equivalence class of \( E \) an arbitrary ensemble \( \{ p_j | \tau_j \rangle \} \) equivalent to \( \mathcal{E}(d_i, |\phi_i \rangle) \); we suppose that the index \( j \) runs from 0 to \( N \) (\( n \)), without excluding the case in which \( N \) is infinite. We know that the fact that the statistical operators associated to such ensembles are identical implies that the normalized states \( |\tau_j \rangle \) are linear combinations of the orthonormal states \( |\phi_i \rangle \):

\[
|\tau_j \rangle = \sum_{i=0}^{n} b_{ji} |\phi_i \rangle, \quad j = 0, 1, ..., N.
\] (2.8)

We define now a rectangular matrix \( V_{ij} \) having \( n + 1 \) rows and \( N + 1 \) columns by putting:

\[
V_{ij} = \sqrt{\frac{p_j}{d_i}} b_{ji}, \quad i = 0, 1, ..., n; \quad j = 0, 1, ..., N.
\] (2.9)

From the relation \( \sum_{i=0}^{n} d_i |\phi_i \rangle \langle \phi_i | = \sum_{j=0}^{N} p_j |\tau_j \rangle \langle \tau_j | \), using Eq. (10) we immediately get:

\[
\sum_{j=0}^{N} p_j b_{ji} b_{jk}^{*} = d_i \delta_{ik}.
\] (2.10)

The above relation implies:

\[
\sum_{j=0}^{N} V_{ij} (V^\dagger)_{jk} = \sum_{j=0}^{N} \frac{p_j}{d_i} \sqrt{\frac{p_j}{d_k}} b_{ji} b_{jk}^{*} = \delta_{ik}.
\] (2.11)

We thus have \( n + 1 \) normalized and orthogonal vectors \( \{ \tilde{w}_r \}, \) \( r = 0, 1, ..., n \) of \( \mathbb{C}^{N+1} \), whose components are the row elements of the matrix \( V_{rj} \):

\[
\tilde{w}_r = (V_{10}, V_{11}, ..., V_{1N}), \quad r = 0, 1, ..., n
\] (2.12)

If \( N \) is finite, we pass from the vectors \( \{ \tilde{w}_r \} \) to new vectors \( \{ w_r \} \) of \( \mathbb{C}^{\infty} \) by considering equal to zero the components of \( \{ \tilde{w}_r \} \) from \( N + 1 \) on. We then extend the set \( \{ w_r \} \) to a complete orthonormal set of \( \mathbb{C}^{\infty} \), by adding appropriately chosen normalized vectors \( \{ w_s \}, \) \( s = n + 1, .., \infty \). Correspondingly, the rectangular matrix \( V_{ij} \) of Eq. (2.9) is transformed into an infinite square matrix, whose rows are the components of the vectors \( \{ w_r \} \), for \( r = 0, 1, .., \infty \). Due to Eq. (2.11) and the procedure we have followed, this infinite square matrix — which we keep calling \( V_{ij} \) — is unitary.

Let us consider now an observable \( \Omega^K \) of \( \mathcal{H}^{K} \) having a purely discrete and non degenerate spectrum with eigenvectors \( |B_j \rangle = V_{ji}^\dagger |A_i \rangle \); this implies that \( |A_i \rangle = V_{ij} |B_j \rangle \). Since \( V_{ij} \) is unitary, we can repeat the previous procedure which amounts simply in replacing, in Eq. (2.3), the states \( |a_i \rangle = |A_i \rangle \) appearing there with their Fourier expansion in terms of the set \( \{ |B_j \rangle \} \). Then Eq. (2.3) takes the form (2.7) where, according to the definition of \( \tilde{\chi}_j \) given in Eq. (2.3) and of \( |\tau_j \rangle \) given in Eq. (2.3):

\[
|\tilde{\chi}_j \rangle = \sum_{i=0}^{n} \sqrt{d_i} V_{ij} |\phi_i \rangle = \sqrt{p_j} \sum_{i=0}^{n} b_{ji} |\phi_i \rangle = \sqrt{p_j} |\tau_j \rangle.
\] (2.13)
This shows that \(|\tilde{\chi}_j\rangle\rangle^2 = p_j\) and that normalizing \(|\tilde{\chi}_j\rangle\rangle\) we get the states \(|\tau_j\rangle\rangle\). Accordingly, Eq. (2.7) becomes:

\[
|\Psi_T\rangle = \sum_{j=0}^{N} \sqrt{p_j} |\tau_j\rangle \otimes |B_j\rangle,
\]

(2.14)

so that measurement of \(\Omega^K\) reduces the state \(|\Psi_T\rangle\rangle\) to the desired ensemble \(E(p_j, |\tau_j\rangle)\). Since \(E(p_j, |\tau_j\rangle)\) is an arbitrary ensemble belonging to the equivalence class \([E(d_i, |\phi_i\rangle)]\), this completes our proof.

The now obtained result shows how, once one has prepared the pure state \(|\Psi_T\rangle\rangle\), he has an immediate complete classification of all ensembles belonging to the equivalence class of \(E(d_i, |\phi_i\rangle)\), an alternative way of deriving the nice result of [3].

Of course, within any equivalence class there are also mixtures which involve a continuous union of pure states i.e.

\[E(p(\lambda), |\phi\rangle) \rightarrow \rho_E = \int d\lambda p(\lambda) |\phi\rangle\langle\phi|,\]

(2.15)

with \(\int d\lambda p(\lambda) = 1\). To get such mixtures from the pure state \(|\Psi\rangle\rangle\) we have, obviously, to measure with infinite precision an observable of \(H^K\) having a continuous spectrum. This is formally but not practically feasible.

Concluding, if we can implement our “von Neumann–like ideal interaction scheme” we can perform the desired purification and then prepare any one of the ensembles in the equivalence class of \(E(d_i, |\phi_i\rangle)\) by performing an appropriate measurement on the system \(K\).

3 The appropriate hamiltonian for the desired purification

To face our problem let us consider the following self-adjoint operator of \(H^{S+K}\):

\[H_j = i |\phi_j\rangle\langle\phi_j| \otimes [|a_0\rangle\langle a_0| - |a_j\rangle\langle a_j|],\]

(3.1)

and let us evaluate its powers. We have:

\[
H_j^{2n+1} = H_j, \\
H_j^{2n} = |\phi_j\rangle\langle\phi_j| \otimes [|a_0\rangle\langle a_0| + |a_j\rangle\langle a_j|].
\]

(3.2)

Let us consider now the operator \(\exp(-i\omega H_j T)\):

\[
\exp(-i\omega H_j T) = \cos(\omega H_j T) - i \sin(\omega H_j T).
\]

(3.3)

Since \(\sin\) contains only odd powers of \(H_j\) we have:

\[
\sin(\omega H_j T) = H_j \sin(\omega T),
\]

(3.4)

while, since all even powers of \(H_j\) equal \(H_j^2\) we can write:

\[
\cos(\omega H_j T) = 1 - H_j^2[-1 + 1 + \frac{1}{2}\omega^2 T^2 - ...] = 1 - H_j^2 + H_j^2 \cos(\omega T).
\]

(3.5)

We now choose for \(T\) a value such that \(\cos(\omega T) = 0, \sin(\omega T) = 1\), getting:

\[
\exp(-i\omega H_j T) = 1 - H_j^2 - iH_j.
\]

(3.6)
The last equation implies that
\[
\exp(-i\omega H_j T) |\phi_j\rangle \otimes |a_0\rangle = [1 - H_j^2 - iH_j] |\phi_j\rangle \otimes |a_0\rangle = |\phi_j\rangle \otimes |a_j\rangle,
\]
(3.7)
as desired.

We remark now that \([H_j, H_k] = 0\) and \(H_k |\phi_j\rangle \otimes |a_0\rangle = 0\) for \(k \neq j\). Accordingly, if consideration is given to the hamiltonian \(H = \sum_{j=0}^{\infty} H_j\) we have:
\[
\exp(-i\omega HT) |\phi_j\rangle \otimes |a_0\rangle = |\phi_j\rangle \otimes |a_j\rangle, \quad \forall j.
\]
(3.8)
Therefore, we have explicitly exhibited an hamiltonian which performs our game, i.e., it leads to the desired purification of our statistical mixture.

Actually, the purification procedure becomes interesting when one can prepare a desired mixture among all those of an equivalence class at–a–distance, as appropriately stressed by Gisin [2]. To reach this goal a very small change in our formalism is necessary. Let us identify the states \(|a_j\rangle\) of our equation with the internal eigenstates of a system (e.g. the stationary states of an hydrogen atom). One can then add to our hamiltonian a term \(\gamma P_{CM}\), where \(\gamma\) is an appropriately chosen c-number and \(P_{CM}\) is the center–of–mass momentum of the system. The evolution induced by the total hamiltonian implies a displacement of the system \(K\) of an amount governed by the value of \(\gamma\), so that in the time interval \(T\) it is brought arbitrarily far from the space region where its interaction with \(S\) took place. In brief, the auxiliary system is far apart and one can actually use the pure state to prepare the desired statistical ensemble of systems \(S\) at–a–distance.

4 A quantum computational example

It is interesting to notice that, for most cases of interest in quantum computational theory, the outlined procedure can be easily implemented by resorting to elementary logical gates. To this purpose, let us suppose that \(S\) is a qubit, i.e. a two–level system, and let us denote as \(|0\rangle, |1\rangle\) the computational basis of \(\mathcal{H}^S\). The controlled–NOT operator acting on qubit \(S\) (taken as the control bit) and on the two–dimensional manifold spanned by the computational basis states \(|a_0\rangle, |a_1\rangle\) of system \(K\) (taken as the target bit) induces precisely the transformation:
\[
|0\rangle \otimes |a_0\rangle \implies |0\rangle \otimes |a_0\rangle
\]
\[
|1\rangle \otimes |a_0\rangle \implies |1\rangle \otimes |a_1\rangle,
\]
(4.1)
which is the desired evolution. In this way, we can purify any statistical ensemble belonging to the equivalence class of
\[
\mathcal{E}(p, |0\rangle; 1 - p, |1\rangle), \quad 0 < p < 1,
\]
(4.2)
by starting with an appropriate superposition analogous to the one of Eq. (2.2).

Let us now consider an arbitrary equivalence class, different from the previous one and containing the ensemble (corresponding to the diagonal form of \(\rho\)):
\[
\mathcal{E}(q, |x_+\rangle; 1 - q, |x_-\rangle), \quad 0 < q < 1,
\]
(4.3)
where \(|x_+\rangle\) and \(|x_-\rangle\) are a basis obtained from the computational basis \(|0\rangle, |1\rangle\) by an appropriate “rotation” of the system:
\[
|x_+\rangle = R_S |0\rangle, \quad |x_-\rangle = R_S |1\rangle.
\]
(4.4)
The circuit that implements the evolution

\[
\begin{align*}
|x_+\rangle \otimes |a_0\rangle & \implies |x_+\rangle \otimes |a_0\rangle, \\
|x_-\rangle \otimes |a_0\rangle & \implies |x_-\rangle \otimes |a_1\rangle,
\end{align*}
\]

leading to the purification of the ensemble, corresponds to a “rotation” \( R_S \) on the control bit, followed by a controlled–NOT gate and by an inverse “rotation” \( R_S \), as shown in the picture.

Thus, the Hamiltonian that induces the desired evolution can be identified with a rotation in \( \mathcal{H}^S \), a controlled–NOT operation in \( \mathcal{H}^S \otimes \mathcal{H}^K \), and finally a counter–rotation in \( \mathcal{H}^S \).

In this way, we have identified the appropriate way to purify any statistical ensemble of the two–dimensional system \( S \). Useless to say, our procedure can be easily generalized to systems containing several qubits and, more in general, to arbitrary quantum systems.

References

[1] M.A. Nielsen and I.L. Chuang, Quantum Computation and Quantum Information, Cambridge University Press, Cambridge (2000).

[2] N. Gisin, Helv. Phys. Acta 62, 363 (1989).

[3] L.P. Hughston, R. Jozsa and W. Wootters, Phys. Lett. A 183, 14 (1993).