Reduced density operator

Masatsugu Sei Suzuki
Department of Physics, SUNY at Binghamton
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Here we discuss the density operator for the two and three-particles system. The concept of the reduced density operator is significant. The reduced density operator enables one to obtain expectation values of one subsystem 1's observables without bothering about the states of the other subsystem 2. It is formed from the density operator of the entire system by taking the **partial trace** over the states of subsystem 2.

1. Kronecker product

A classical bit of information is represented by a system that can be in either of two states, 0, 1. At the quantum mechanical level, the most natural candidate for replacing a classical bit is the state of a two-level system, whose basic components may be written as

$$|\psi_1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = |0\rangle, \qquad |\psi_2\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} = |1\rangle$$

This is the so-called quantum bit of information, or, in short, a qubit. Here we define the combined state of two qubits as

$$|\psi_1\rangle \otimes |\psi_2\rangle = \text{KroneckerProduct}[\psi_1,\ \psi_2]$$

Then we have

$$|0\rangle \otimes |0\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \qquad |0\rangle \otimes |1\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \qquad |1\rangle \otimes |0\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}$$

$$|1\rangle \otimes |1\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

$$|0\rangle \otimes |0\rangle)(\langle 0| \otimes \langle 0| = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix},$$

$$|0\rangle \otimes |1\rangle)(\langle 0| \otimes \langle 1| = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

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2. Calculation of density operator by Mathematica

A classical bit of information is represented by a system that can be in either of two states, 0, 1. At the quantum mechanical level, the most natural candidate for replacing a classical bit is the state of a two-level system, whose basic components may be written as

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The Kronecker product

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((**Note**))

$$\begin{aligned} |1\rangle \otimes |0\rangle)(\langle 0| \otimes \langle 1| &= (|1\rangle\langle 0|)_1 \otimes (|0\rangle\langle 1|)_2 \\ &= \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \otimes \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \\ &= \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \end{aligned}$$

$$\begin{aligned} |1\rangle \otimes |1\rangle)(\langle 1| \otimes \langle 1| &= (|1\rangle\langle 1|)_1 \otimes (|1\rangle\langle 1|)_2 \\ &= \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \\ &= \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \end{aligned}$$

3. Density operators for two-particle system

We consider the two-particle system. Typical example is the two-spin system with spin 1/2. There are four states,

$$|+z,+z\rangle = |+z\rangle_1 \otimes |+z\rangle_2, \qquad |+z,-z\rangle = |+z\rangle_1 \otimes |-z\rangle_2$$

$$|-z,+z\rangle = |-z\rangle_1 \otimes |+z\rangle_2 , \qquad |-z,-z\rangle = |-z\rangle_1 \otimes |-z\rangle_2 .$$

In general, the density operator for two particle system can be expressed by

$$\begin{aligned}
\hat{\rho}_{12} &= \sum_{i,j,k,l} |i,j\rangle\langle i,j|\hat{\rho}|k,l\rangle\langle k,l| \\
&= \sum_{i,j,k,l} \langle i,j|\hat{\rho}|k,l\rangle (|\phi_i\rangle \otimes |\chi_j\rangle)(\langle\phi_k| \otimes \langle\chi_l|) \\
&= \sum_{i,j,k,l} \langle i,j|\hat{\rho}|k,l\rangle (|\phi_i\rangle\langle\phi_k|) \otimes (|\chi_j\rangle\langle\chi_l|)
\end{aligned}$$

where $|\phi_i\rangle$ is the eigenket of the particle 1 and $|\chi_j\rangle$ is the eigenket of the particle 2. $\langle i,j|\hat{\rho}|k,l\rangle$ is the density matrix. Here we use the formula

$$Tr_1(|\phi_i\rangle\langle\phi_k|)_1 \otimes (|\chi_j\rangle\langle\chi_l|)_2 = \langle\phi_k|\phi_i\rangle(|\chi_j\rangle\langle\chi_l|)_2 = \delta_{k,i}(|\chi_j\rangle\langle\chi_l|)_2$$

$$Tr_2(|\phi_i\rangle \otimes |\chi_j\rangle)(\langle\phi_k| \otimes \langle\chi_l|) = \langle\chi_l|\chi_j\rangle(|\phi_i\rangle\langle\phi_k|)_1 = \delta_{l,j}(|\phi_i\rangle\langle\phi_k|)_1$$

where

$$\begin{aligned}
Tr_1(|\phi_i\rangle\langle\phi_k|)_1 &= \sum_l \langle\phi_l|\phi_i\rangle\langle\phi_k|\phi_l\rangle \\
&= \sum_l \langle\phi_k|\phi_l\rangle\langle\phi_l|\phi_i\rangle \\
&= \langle\phi_k|\phi_i\rangle
\end{aligned}$$

and

$$\begin{aligned}
Tr_2(|\chi_j\rangle\langle\chi_l|)_2 &= \sum_k \langle\chi_k|\chi_j\rangle\langle\chi_l|\chi_k\rangle \\
&= \sum_k \langle\chi_l|\chi_k\rangle\langle\chi_k|\chi_j\rangle \\
&= \langle\chi_l|\chi_j\rangle
\end{aligned}$$

4. Reduced density operator $\hat{\rho}_1$

The reduced density operator $\hat{\rho}_1$ describes completely all the properties/outcomes of measurements of the system 1, given that system 2 is left unobserved ("tracing out" system 2).

This represent the maximum information which is available about the particle 1 alone, irrespective of the state of particle 2. The reduced density operator $\hat{\rho}_1$ is defined as

$$\begin{aligned}
\hat{\rho}_1 &= Tr_2[\hat{\rho}_{12}] \\
&= \sum_{i,j,k,l} \langle i,j|\hat{\rho}|k,l\rangle (|\phi_i\rangle\langle\phi_k|) Tr_2[(|\chi_j\rangle\langle\chi_l|] \\
&= \sum_{i,j,k,l} \langle i,j|\hat{\rho}|k,l\rangle (|\phi_i\rangle\langle\phi_k|) \langle\chi_l|\chi_j\rangle \\
&= \sum_{i,j,k,l} \langle i,j|\hat{\rho}|k,l\rangle (|\phi_i\rangle\langle\phi_k|) \delta_{l,j} \\
&= \sum_{i,j,k} \langle i,j|\hat{\rho}|k,j\rangle |\phi_i\rangle\langle\phi_k|
\end{aligned}$$

where we use the formula

$$Tr_2[(|\chi_j\rangle\langle\chi_l|] = \langle\chi_l|\chi_j\rangle = \delta_{l,j}.$$

Note that

$$\begin{aligned}
\hat{\rho}_1 &= [\langle 1,1|\hat{\rho}|1,1\rangle + \langle 1,2|\hat{\rho}|1,2\rangle]|\phi_1\rangle\langle\phi_1| \\
&\quad + \langle 1,1|\hat{\rho}|2,1\rangle + \langle 1,2|\hat{\rho}|2,2\rangle]|\phi_1\rangle\langle\phi_2| \\
&\quad + \langle 2,1|\hat{\rho}|1,1\rangle + \langle 2,2|\hat{\rho}|1,2\rangle]|\phi_2\rangle\langle\phi_1| \\
&\quad + \langle 2,1|\hat{\rho}|2,1\rangle + \langle 2,2|\hat{\rho}|2,2\rangle]|\phi_2\rangle\langle\phi_2|] \\
&= \begin{pmatrix} \langle 1,1|\hat{\rho}|1,1\rangle & \langle 1,1|\hat{\rho}|2,1\rangle \\ \langle 2,1|\hat{\rho}|1,1\rangle & \langle 2,1|\hat{\rho}|2,1\rangle \end{pmatrix} + \begin{pmatrix} \langle 1,2|\hat{\rho}|1,2\rangle & \langle 1,2|\hat{\rho}|2,2\rangle \\ \langle 2,2|\hat{\rho}|1,2\rangle & \langle 2,2|\hat{\rho}|2,2\rangle \end{pmatrix} \\
&= \begin{pmatrix} \langle 1,1|\hat{\rho}|1,1\rangle + \langle 1,2|\hat{\rho}|1,2\rangle & \langle 1,1|\hat{\rho}|2,1\rangle + \langle 1,2|\hat{\rho}|2,2\rangle \\ \langle 2,1|\hat{\rho}|1,1\rangle + \langle 2,2|\hat{\rho}|1,2\rangle & \langle 2,1|\hat{\rho}|2,1\rangle + \langle 2,2|\hat{\rho}|2,2\rangle \end{pmatrix}
\end{aligned}$$

for the two-particles system. For simplicity we use the following notation.

$$\hat{\rho}_1 = Tr_2[\hat{\rho}] = \begin{pmatrix} \rho_{11} & \rho_{13} \\ \rho_{31} & \rho_{33} \end{pmatrix} + \begin{pmatrix} \rho_{22} & \rho_{24} \\ \rho_{42} & \rho_{44} \end{pmatrix} = \begin{pmatrix} \rho_{11} + \rho_{22} & \rho_{13} + \rho_{24} \\ \rho_{31} + \rho_{42} & \rho_{33} + \rho_{44} \end{pmatrix}$$

where $|1,1\rangle = |1\rangle$, $|1,2\rangle = |2\rangle$, $|2,1\rangle = |3\rangle$, $|2,2\rangle = |4\rangle$,

$\langle ++\|\rho\|++\rangle$	$\langle ++\|\rho\|+-\rangle$	$\langle ++\|\rho\|-+\rangle$	$\langle ++\|\rho\|--\rangle$
$\langle +-\|\rho\|++\rangle$	$\langle +-\|\rho\|+-\rangle$	$\langle +-\|\rho\|-+\rangle$	$\langle +-\|\rho\|--\rangle$
$\langle -+\|\rho\|++\rangle$	$\langle -+\|\rho\|+-\rangle$	$\langle -+\|\rho\|-+\rangle$	$\langle -+\|\rho\|--\rangle$
$\langle --\|\rho\|++\rangle$	$\langle --\|\rho\|+-\rangle$	$\langle --\|\rho\|-+\rangle$	$\langle --\|\rho\|--\rangle$

5. Reduced density operator $\hat{\rho}_2$

The reduced density operator $\hat{\rho}_2$ describes completely all the properties/outcomes of measurements of the system 2, given that system 1 is left unobserved ("tracing out" system 1). This represent the maximum information which is available about the particle 2 alone, irrespective of the state of particle 1.

The reduced density operator $\hat{\rho}_2$ is defined by

$$
\begin{aligned}
\hat{\rho}_2 &= Tr_1[\hat{\rho}_{12}] \\
&= \sum_{i,j,k,l} \langle i,j|\hat{\rho}|k,l\rangle (|\chi_j\rangle\langle\chi_l|) Tr_1[(|\phi_i\rangle\langle\phi_k|)] \\
&= \sum_{i,j,,l} \langle i,j|\hat{\rho}|k,l\rangle |\chi_j\rangle\langle\chi_l|\delta_{i,k} \\
&= \sum_{i,j,l} \langle i,j|\hat{\rho}|i,l\rangle |\chi_j\rangle\langle\chi_l|
\end{aligned}
$$

We note that

$$\begin{aligned}\hat{\rho}_2 &= [\langle 1,1|\hat{\rho}|1,1\rangle + \langle 2,1|\hat{\rho}|2,1\rangle]|\chi_1\rangle\langle\chi_1| \\ &\quad + \langle 1,1|\hat{\rho}|1,2\rangle + \langle 2,1|\hat{\rho}|2,2\rangle]|\chi_1\rangle\langle\chi_2| \\ &\quad + \langle 1,2|\hat{\rho}|1,1\rangle + \langle 2,2|\hat{\rho}|2,1\rangle]|\chi_2\rangle\langle\chi_1| \\ &\quad + \langle 1,2|\hat{\rho}|1,2\rangle + \langle 2,2|\hat{\rho}|2,2\rangle]|\chi_2\rangle\langle\chi_2|] \\ &= \langle 1,1|\hat{\rho}|1,1\rangle + \langle 2,1|\hat{\rho}|2,1\rangle]\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \\ &\quad + \langle 1,1|\hat{\rho}|1,2\rangle + \langle 2,1|\hat{\rho}|2,2\rangle]\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \\ &\quad + \langle 1,2|\hat{\rho}|1,1\rangle + \langle 2,2|\hat{\rho}|2,1\rangle]\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \\ &\quad + \langle 1,2|\hat{\rho}|1,2\rangle + \langle 2,2|\hat{\rho}|2,2\rangle]\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \\ &= \begin{pmatrix} \langle 1,1|\hat{\rho}|1,1\rangle & \langle 1,1|\hat{\rho}|1,2\rangle \\ \langle 1,2|\hat{\rho}|1,1\rangle & \langle 1,2|\hat{\rho}|1,2\rangle \end{pmatrix} + \begin{pmatrix} \langle 2,1|\hat{\rho}|2,1\rangle & \langle 2,1|\rho|2,2\rangle \\ \langle 2,2|\hat{\rho}|2,1\rangle & \langle 2,2|\hat{\rho}|2,2\rangle \end{pmatrix} \\ &= \begin{pmatrix} \langle 1,1|\hat{\rho}|1,1\rangle + \langle 2,1|\hat{\rho}|2,1\rangle & \langle 1,1|\rho|1,2\rangle + \langle 2,1|\hat{\rho}|2,2\rangle \\ \langle 1,2|\hat{\rho}|1,1\rangle + \langle 2,2|\hat{\rho}|2,1\rangle & \langle 1,2|\hat{\rho}|1,2\rangle + \langle 2,2|\hat{\rho}|2,2\rangle \end{pmatrix}\end{aligned}$$

for the two-particles system. For simplicity, we use the following notation

$$\hat{\rho}_2 = Tr_1[\hat{\rho}] = \begin{pmatrix} \rho_{11} & \rho_{12} \\ \rho_{21} & \rho_{22} \end{pmatrix} + \begin{pmatrix} \rho_{33} & \rho_{34} \\ \rho_{43} & \rho_{44} \end{pmatrix} = \begin{pmatrix} \rho_{11} + \rho_{33} & \rho_{12} + \rho_{34} \\ \rho_{21} + \rho_{43} & \rho_{22} + \rho_{44} \end{pmatrix}$$

<++|ρ|++>   <++|ρ|+−>   <++|ρ|−+>   <++|ρ|−−>

<+−|ρ|++>   <+−|ρ|+−>   <+−|ρ|−+>   <+−|ρ|−−>

<−+|ρ|++>   <−+|ρ|+−>   <−+|ρ|−+>   <−+|ρ|−−>

<−−|ρ|++>   <−−|ρ|+−>   <−−|ρ|−+>   <−−|ρ|−−>

6. Example-1: two spins (independent subsystems)

We consider the state of the composite system 1-2 consisting of independent subsystems

$$\left|\psi_{12}\right\rangle = \frac{1}{\sqrt{2}}(\left|+z,1\right\rangle + \left|-z,1\right\rangle) \otimes \left|+z,2\right\rangle = \left|+x,1\right\rangle \otimes \left|+z,2\right\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\1\\0\end{pmatrix}$$

The density operator is obtained as

$$\begin{aligned}\hat{\rho}_{12} &= \left|\psi_{12}\right\rangle\left\langle\psi_{12}\right| \\ &= (\left|+x,1\right\rangle \otimes \left|+z,2\right\rangle)(\left\langle +x,1\right| \otimes \left\langle +z,2\right|) \\ &= (\left|+x,1\right\rangle\left\langle +x,1\right|) \otimes (\left|+z,2\right\rangle\left\langle +z,2\right|) \\ &= \hat{\rho}_A \otimes \hat{\rho}_B\end{aligned}$$

where $\hat{\rho}_A$ and $\hat{\rho}_B$ denote the operators for particle-1 and particle-2, respectively. The matrix form of $\hat{\rho}_{12}$ is given by

$$\hat{\rho}_{12} = \frac{1}{2}\begin{pmatrix} 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

The reduce density operators $\hat{\rho}_1$ and $\hat{\rho}_2$ are obtained as

$$\hat{\rho}_2 = Tr_1[\hat{\rho}_{12}] = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} = \hat{\rho}_B$$

$$\hat{\rho}_1 = Tr_2[\hat{\rho}_{12}] = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} + \frac{1}{2}\begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} = \hat{\rho}_A$$

Note that

$$\hat{\rho}_2 = Tr_1[\hat{\rho}_{12}] = Tr_A[\hat{\rho}_A \otimes \hat{\rho}_B] = \hat{\rho}_B Tr_A[\hat{\rho}_A] = \hat{\rho}_B$$

$$\hat{\rho}_1 = Tr_2[\hat{\rho}_{12}] = Tr_B[\hat{\rho}_A \otimes \hat{\rho}_B] = \hat{\rho}_A Tr_B[\hat{\rho}_B] = \hat{\rho}_A$$

using the formula given in the APPENDIX-II

7. **Example-2**: Two spins: independent subsystems

We start with the two-particle pure state $|\psi_{12}\rangle = |+z,1\rangle|+z,2\rangle$. The density operator is given by

$$\begin{aligned}
\hat{\rho}_{12} &= (|+z,1\rangle \otimes |+z,2\rangle)(\langle +z;1| \otimes \langle +z,2|) \\
&= (|+z,1\rangle\langle +z;1| \otimes |+z,2\rangle\langle +z,2|) \\
&= \hat{\rho}_A \otimes \hat{\rho}_B \\
&= \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}
\end{aligned}$$

under the basis of {$|+z\rangle$ and $|-z\rangle$ }, where

$$\hat{\rho}_A = \hat{\rho}_B = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

The reduced density is obtained as

$$\hat{\rho}_1 = Tr_2[\hat{\rho}_{12}] = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} = \hat{\rho}_A$$

$$\hat{\rho}_2 = Tr_1[\hat{\rho}_{12}] = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} = \hat{\rho}_B$$

under the basis of $\{ \left| + \right\rangle, \left| - \right\rangle \}$.

8. Example-3: Bell's two-particle entangled state

The Bell's entangled state is given by

$$\left| \Psi_{12}{}^{(-)} \right\rangle = \frac{1}{\sqrt{2}} [\left| +z;1 \right\rangle \left| -z;2 \right\rangle - \left| -z;1 \right\rangle \left| +z;2 \right\rangle]$$

The density operator (in the pure state) is given by

$$\hat{\rho}_{12} = \left| \Psi_{12}{}^{(-)} \right\rangle \left\langle \Psi_{12}{}^{(-)} \right| = \frac{1}{2} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

((**Mathematica**))

```
ψ1 = (1
      0); ψ2 = (0
                1);
ψ12 =
  1/√2 (KroneckerProduct[ψ1, ψ2] -
      KroneckerProduct[ψ2, ψ1]) // Simplify
```

$$\left\{\{0\}, \left\{\frac{1}{\sqrt{2}}\right\}, \left\{-\frac{1}{\sqrt{2}}\right\}, \{0\}\right\}$$

```
ρ0 = ψ12.Transpose[ψ12] // Simplify;
ρ0 // MatrixForm
```

$$\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & -\frac{1}{2} & 0 \\ 0 & -\frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

The reduced density operator is obtained as

$$\hat{\rho}_1 = Tr_2[\rho_{12}] = \frac{1}{2}\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} + \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$\hat{\rho}_2 = Tr_1[\rho_{12}] = \frac{1}{2}\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} + \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

under the basis of $\{\left|+z\right\rangle, \left|-z\right\rangle\}$. Thus for measurements of particle 1 (or 2) the Bell's state behaves like the mixed states of completely un-polarized ensemble.

((Note))
M.A Nielsen and I.L. Chuang, Quantum computation and quantum information, 10th Anniversary Edition (Cambridge, 2010).

Notice that this state $\hat{\rho}_1$ (or $\hat{\rho}_2$) is a mixed state. This is a quite remarkable result. The state of the joint system of two qubits is a pure state, that is, it is known exactly, however, the first qubit is in a mixed state, that is a state about which we apparently do not have maximal knowledge. This strange property, that the joint state of a system can be completely known, yet a subsystem be in the mixed state, is another hallmark of quantum entanglement.

9. Density operator for three-spins system

In general, the density operator for three particle system can be expressed by

$$\begin{aligned}
\hat{\rho}_{123} &= \sum_{\substack{i,j,k,l,\\ m,n}} \left|i,j,k\right\rangle\left\langle i,j,k\right|\hat{\rho}\left|l,m,n\right\rangle\left\langle l,m,n\right| \\
&= \sum_{\substack{i,j,k,l,\\ m,n}} \left\langle i,j,k\right|\hat{\rho}\left|l,m,n\right\rangle (\left|\phi_i\right\rangle \otimes \left|\chi_j\right\rangle \otimes \left|\eta_k\right\rangle)(\left\langle\phi_l\right| \otimes \left\langle\chi_m\right| \otimes \left\langle\eta_n\right|) \\
&= \sum_{\substack{i,j,k,l,\\ m,n}} \left\langle i,j,k\right|\hat{\rho}\left|l,m,n\right\rangle (\left|\phi_i\right\rangle\left\langle\phi_l\right|)_1 \otimes (\left|\chi_j\right\rangle\left\langle\chi_m\right|)_2 \otimes (\left|\eta_k\right\rangle\left\langle\eta_n\right|)_3
\end{aligned}$$

where $\left|\phi_i\right\rangle$ is the eigenket of the particle 1, and $\left|\chi_j\right\rangle$ is the eigenket of the particle 2, and $\left|\eta_k\right\rangle$ is the eigenket of the particle 3. $\left\langle i,j,k\right|\hat{\rho}\left|l,m,n\right\rangle$ is the density matrix. Here we use the formula

$$\begin{aligned}
Tr_1(\left|\phi_i\right\rangle\left\langle\phi_l\right|)_1 \otimes (\left|\chi_j\right\rangle\left\langle\chi_m\right|)_2 \otimes (\left|\eta_k\right\rangle\left\langle\eta_n\right|)_3 &= \left\langle\phi_l|\phi_i\right\rangle(\left|\chi_j\right\rangle\left\langle\chi_m\right|)_2 \otimes (\left|\eta_k\right\rangle\left\langle\eta_n\right|)_3 \\
&= \delta_{l,i}(\left|\chi_j\right\rangle\left\langle\chi_m\right|)_2 \otimes (\left|\eta_k\right\rangle\left\langle\eta_n\right|)_3
\end{aligned}$$

$$\begin{aligned}
Tr_2(\left|\phi_i\right\rangle\left\langle\phi_l\right|)_1 \otimes (\left|\chi_j\right\rangle\left\langle\chi_m\right|)_2 \otimes (\left|\eta_k\right\rangle\left\langle\eta_n\right|)_3 &= \left\langle\chi_m|\chi_j\right\rangle(\left|\phi_i\right\rangle\left\langle\phi_l\right|)_1 \otimes (\left|\eta_k\right\rangle\left\langle\eta_n\right|)_3 \\
&= \delta_{m,j}(\left|\phi_i\right\rangle\left\langle\phi_l\right|)_1 \otimes (\left|\eta_k\right\rangle\left\langle\eta_n\right|)_3
\end{aligned}$$

$$\begin{aligned}
Tr_3(\left|\phi_i\right\rangle\left\langle\phi_l\right|)_1 \otimes (\left|\chi_j\right\rangle\left\langle\chi_m\right|)_2 \otimes (\left|\eta_k\right\rangle\left\langle\eta_n\right|)_3 &= \left\langle\eta_n|\eta_k\right\rangle(\left|\phi_i\right\rangle\left\langle\phi_l\right|)_1 \otimes (\left|\chi_j\right\rangle\left\langle\chi_m\right|)_2 \\
&= \delta_{n,k}(\left|\phi_i\right\rangle\left\langle\phi_l\right|)_1 \otimes (\left|\chi_j\right\rangle\left\langle\chi_m\right|)_2
\end{aligned}$$

We consider the density operator for the three-spins system (with spin 1/2).

$$\hat{\rho}_{123} = \begin{pmatrix}
\rho_{11} & \rho_{12} & \rho_{13} & \rho_{14} & \rho_{15} & \rho_{16} & \rho_{17} & \rho_{18} \\
\rho_{21} & \rho_{22} & \rho_{23} & \rho_{24} & \rho_{25} & \rho_{26} & \rho_{27} & \rho_{18} \\
\rho_{31} & \rho_{32} & \rho_{33} & \rho_{34} & \rho_{35} & \rho_{36} & \rho_{37} & \rho_{18} \\
\rho_{41} & \rho_{42} & \rho_{43} & \rho_{44} & \rho_{45} & \rho_{46} & \rho_{47} & \rho_{18} \\
\rho_{51} & \rho_{52} & \rho_{53} & \rho_{54} & \rho_{55} & \rho_{56} & \rho_{57} & \rho_{18} \\
\rho_{61} & \rho_{62} & \rho_{63} & \rho_{64} & \rho_{65} & \rho_{66} & \rho_{67} & \rho_{18} \\
\rho_{71} & \rho_{72} & \rho_{73} & \rho_{74} & \rho_{75} & \rho_{76} & \rho_{77} & \rho_{78} \\
\rho_{81} & \rho_{82} & \rho_{83} & \rho_{84} & \rho_{85} & \rho_{86} & \rho_{87} & \rho_{88}
\end{pmatrix}$$

where

$$\rho_{11} = \langle +++|\hat{\rho}|+++\rangle, \qquad \rho_{12} = \langle +++|\hat{\rho}|++-\rangle,$$

$$\rho_{13} = \langle +++|\hat{\rho}|+-+\rangle, \qquad \rho_{14} = \langle +++|\hat{\rho}|+--\rangle$$

$$\rho_{15} = \langle +++|\hat{\rho}|-++\rangle, \qquad \rho_{16} = \langle +++|\hat{\rho}|-+-\rangle,$$

$$\rho_{17} = \langle +++|\hat{\rho}|--+\rangle, \qquad \rho_{18} = \langle +++|\hat{\rho}|---\rangle$$

and so on.

10. Reduced density operator

The reduced density operator $\hat{\rho}_{23}$ is obtained from the full density operator by tracing over the diagonal matrix elements of particle 1, leading to

$$\begin{aligned}\hat{\rho}_{23} &= Tr_1\hat{\rho} \\ &= \begin{pmatrix} \rho_{11} & \rho_{12} & \rho_{13} & \rho_{14} \\ \rho_{21} & \rho_{22} & \rho_{23} & \rho_{24} \\ \rho_{31} & \rho_{32} & \rho_{33} & \rho_{34} \\ \rho_{41} & \rho_{42} & \rho_{43} & \rho_{44} \end{pmatrix} + \begin{pmatrix} \rho_{55} & \rho_{56} & \rho_{57} & \rho_{58} \\ \rho_{65} & \rho_{66} & \rho_{67} & \rho_{68} \\ \rho_{75} & \rho_{76} & \rho_{77} & \rho_{78} \\ \rho_{85} & \rho_{86} & \rho_{87} & \rho_{88} \end{pmatrix} \\ &= \begin{pmatrix} \chi_{11} & \chi_{12} & \chi_{13} & \chi_{14} \\ \chi_{21} & \chi_{22} & \chi_{23} & \chi_{24} \\ \chi_{31} & \chi_{32} & \chi_{33} & \chi_{34} \\ \chi_{41} & \chi_{42} & \chi_{43} & \chi_{44} \end{pmatrix}\end{aligned}$$

The reduced density operator $\hat{\rho}_3$ is obtained from the full density operator by tracing over the diagonal matrix elements of particles 1 and 2, leading to

$$\begin{aligned}\hat{\rho}_3 &= Tr_2\hat{\rho}_{23} = Tr_{1,2}\hat{\rho} \\ &= \begin{pmatrix} \chi_{11} & \chi_{12} \\ \chi_{21} & \chi_{22} \end{pmatrix} + \begin{pmatrix} \chi_{33} & \chi_{34} \\ \chi_{43} & \chi_{44} \end{pmatrix}\end{aligned}$$

We also have the density operator for the three spins and its reduced density operator

((Reduced density operator $\hat{\rho}_{23}$))

$$\hat{\rho}_{23} = Tr_1[\hat{\rho}] = \begin{pmatrix} \rho_{11} & \rho_{12} & \rho_{13} & \rho_{14} \\ \rho_{21} & \rho_{22} & \rho_{23} & \rho_{24} \\ \rho_{31} & \rho_{32} & \rho_{33} & \rho_{34} \\ \rho_{41} & \rho_{42} & \rho_{43} & \rho_{44} \end{pmatrix} + \begin{pmatrix} \rho_{55} & \rho_{56} & \rho_{57} & \rho_{58} \\ \rho_{65} & \rho_{66} & \rho_{67} & \rho_{68} \\ \rho_{75} & \rho_{76} & \rho_{77} & \rho_{78} \\ \rho_{85} & \rho_{86} & \rho_{87} & \rho_{88} \end{pmatrix}$$

<+++|ρ|+++>	<+++|ρ|++−>	<+++|ρ|+−+>	<+++|ρ|+−−>	<+++|ρ|−++>	<+++|ρ|−+−>	<+++|ρ|−−+>	<+++|ρ|−−−>
<++−|ρ|+++>	<++−|ρ|++−>	<++−|ρ|+−+>	<++−|ρ|+−−>	<++−|ρ|−++>	<++−|ρ|−+−>	<++−|ρ|−−+>	<++−|ρ|−−−>
<+−+|ρ|+++>	<+−+|ρ|++−>	<+−+|ρ|+−+>	<+−+|ρ|+−−>	<+−+|ρ|−++>	<+−+|ρ|−+−>	<+−+|ρ|−−+>	<+−+|ρ|−−−>
<+−−|ρ|+++>	<+−−|ρ|++−>	<+−−|ρ|+−+>	<+−−|ρ|+−−>	<+−−|ρ|−++>	<+−−|ρ|−+−>	<+−−|ρ|−−+>	<+−−|ρ|−−−>
<−++|ρ|+++>	<−++|ρ|++−>	<−++|ρ|+−+>	<−++|ρ|+−−>	<−++|ρ|−++>	<−++|ρ|−+−>	<−++|ρ|−−+>	<−+−|ρ|−−−>
<−+−|ρ|+++>	<−+−|ρ|++−>	<−+−|ρ|+−+>	<−+−|ρ|+−−>	<−+−|ρ|−++>	<−+−|ρ|−+−>	<−+−|ρ|−−+>	<−+−|ρ|−−−>
<−−+|ρ|+++>	<−−+|ρ|++−>	<−−+|ρ|+−+>	<−−+|ρ|+−−>	<−−+|ρ|−++>	<−−+|ρ|−+−>	<−−+|ρ|−−+>	<−−+|ρ|−−−>
<−−−|ρ|+++>	<−−−|ρ|++−>	<−−−|ρ|+−+>	<−−−|ρ|+−−>	<−−−|ρ|−++>	<−−−|ρ|−+−>	<−−−|ρ|−−+>	<−−−|ρ|−−−>

((Reduced density operator $\hat{\rho}_{13}$))

$$\hat{\rho}_{13} = Tr_2[\hat{\rho}] = \begin{pmatrix} \rho_{11} & \rho_{12} & \rho_{15} & \rho_{16} \\ \rho_{21} & \rho_{22} & \rho_{25} & \rho_{26} \\ \rho_{51} & \rho_{52} & \rho_{55} & \rho_{56} \\ \rho_{61} & \rho_{62} & \rho_{65} & \rho_{66} \end{pmatrix} + \begin{pmatrix} \rho_{33} & \rho_{34} & \rho_{37} & \rho_{38} \\ \rho_{43} & \rho_{44} & \rho_{47} & \rho_{48} \\ \rho_{73} & \rho_{74} & \rho_{77} & \rho_{78} \\ \rho_{83} & \rho_{84} & \rho_{87} & \rho_{88} \end{pmatrix}$$

$\langle +++\|\rho\|+++\rangle$	$\langle +++\|\rho\|++-\rangle$	$\langle +++\|\rho\|+-+\rangle$	$\langle +++\|\rho\|+--\rangle$	$\langle +++\|\rho\|-++\rangle$	$\langle +++\|\rho\|-+-\rangle$	$\langle +++\|\rho\|--+\rangle$	$\langle +++\|\rho\|---\rangle$
$\langle ++-\|\rho\|+++\rangle$	$\langle ++-\|\rho\|++-\rangle$	$\langle ++-\|\rho\|+-+\rangle$	$\langle ++-\|\rho\|+--\rangle$	$\langle ++-\|\rho\|-++\rangle$	$\langle ++-\|\rho\|-+-\rangle$	$\langle ++-\|\rho\|--+\rangle$	$\langle ++-\|\rho\|---\rangle$
$\langle +-+\|\rho\|+++\rangle$	$\langle +-+\|\rho\|++-\rangle$	$\langle +-+\|\rho\|+-+\rangle$	$\langle +-+\|\rho\|+--\rangle$	$\langle +-+\|\rho\|-++\rangle$	$\langle +-+\|\rho\|-+-\rangle$	$\langle +-+\|\rho\|--+\rangle$	$\langle +-+\|\rho\|---\rangle$
$\langle +--\|\rho\|+++\rangle$	$\langle +--\|\rho\|++-\rangle$	$\langle +--\|\rho\|+-+\rangle$	$\langle +--\|\rho\|+--\rangle$	$\langle +--\|\rho\|-++\rangle$	$\langle +--\|\rho\|-+-\rangle$	$\langle +--\|\rho\|--+\rangle$	$\langle +--\|\rho\|---\rangle$
$\langle -++\|\rho\|+++\rangle$	$\langle -++\|\rho\|++-\rangle$	$\langle -++\|\rho\|+-+\rangle$	$\langle -++\|\rho\|+--\rangle$	$\langle -++\|\rho\|-++\rangle$	$\langle -++\|\rho\|-+-\rangle$	$\langle -++\|\rho\|--+\rangle$	$\langle -++\|\rho\|---\rangle$
$\langle -+-\|\rho\|+++\rangle$	$\langle -+-\|\rho\|++-\rangle$	$\langle -+-\|\rho\|+-+\rangle$	$\langle -+-\|\rho\|+--\rangle$	$\langle -+-\|\rho\|-++\rangle$	$\langle -+-\|\rho\|-+-\rangle$	$\langle -+-\|\rho\|--+\rangle$	$\langle -+-\|\rho\|---\rangle$
$\langle --+\|\rho\|+++\rangle$	$\langle --+\|\rho\|++-\rangle$	$\langle --+\|\rho\|+-+\rangle$	$\langle --+\|\rho\|+--\rangle$	$\langle --+\|\rho\|-++\rangle$	$\langle --+\|\rho\|-+-\rangle$	$\langle --+\|\rho\|--+\rangle$	$\langle --+\|\rho\|---\rangle$
$\langle ---\|\rho\|+++\rangle$	$\langle ---\|\rho\|++-\rangle$	$\langle ---\|\rho\|+-+\rangle$	$\langle ---\|\rho\|+--\rangle$	$\langle ---\|\rho\|-++\rangle$	$\langle ---\|\rho\|-+-\rangle$	$\langle ---\|\rho\|--+\rangle$	$\langle ---\|\rho\|---\rangle$

((Reduced density operator $\hat{\rho}_{12}$))

$$\hat{\rho}_{12} = Tr_3[\hat{\rho}] = \begin{pmatrix} \rho_{11} & \rho_{13} & \rho_{15} & \rho_{17} \\ \rho_{31} & \rho_{33} & \rho_{35} & \rho_{37} \\ \rho_{51} & \rho_{53} & \rho_{55} & \rho_{57} \\ \rho_{71} & \rho_{73} & \rho_{75} & \rho_{77} \end{pmatrix} + \begin{pmatrix} \rho_{22} & \rho_{24} & \rho_{26} & \rho_{28} \\ \rho_{42} & \rho_{44} & \rho_{46} & \rho_{48} \\ \rho_{62} & \rho_{64} & \rho_{66} & \rho_{68} \\ \rho_{82} & \rho_{84} & \rho_{86} & \rho_{88} \end{pmatrix}$$

<+++|ρ|+++>	<+++|ρ|++->	<+++|ρ|+-+>	<+++|ρ|+-->	<+++|ρ|-++>	<+++|ρ|-+->	<+++|ρ|--+>	<+++|ρ|--->
<++-|ρ|+++>	<++-|ρ|++->	<++-|ρ|+-+>	<++-|ρ|+-->	<++-|ρ|-++>	<++-|ρ|-+->	<++-|ρ|--+>	<++-|ρ|--->
<+-+|ρ|+++>	<+-+|ρ|++->	<+-+|ρ|+-+>	<+-+|ρ|+-->	<+-+|ρ|-++>	<+-+|ρ|-+->	<+-+|ρ|--+>	<+-+|ρ|--->
<+--|ρ|+++>	<+--|ρ|++->	<+--|ρ|+-+>	<+--|ρ|+-->	<+--|ρ|-++>	<+--|ρ|-+->	<+--|ρ|--+>	<+--|ρ|--->
<-++|ρ|+++>	<-++|ρ|++->	<-++|ρ|+-+>	<-++|ρ|+-->	<-++|ρ|-++>	<-++|ρ|-+->	<-++|ρ|--+>	<-++|ρ|--->
<-+-|ρ|+++>	<-+-|ρ|++->	<-+-|ρ|+-+>	<-+-|ρ|+-->	<-+-|ρ|-++>	<-+-|ρ|-+->	<-+-|ρ|--+>	<-+-|ρ|--->
<--+|ρ|+++>	<--+|ρ|++->	<--+|ρ|+-+>	<--+|ρ|+-->	<--+|ρ|-++>	<--+|ρ|-+->	<--+|ρ|--+>	<--+|ρ|--->
<---|ρ|+++>	<---|ρ|++->	<---|ρ|+-+>	<---|ρ|+-->	<---|ρ|-++>	<---|ρ|-+->	<---|ρ|--+>	<---|ρ|--->

11. Example-1 Entangled GHS state

$$\left|\psi_{GHZ}{}^{(+)}\right\rangle = \frac{1}{\sqrt{2}}[\left|+++\right\rangle + \left|---\right\rangle]$$

The density operator is defined by

$$\hat{\rho}_{123} = \left|\psi_{GHZ}{}^{(+)}\right\rangle \left\langle\psi_{GHZ}{}^{(+)}\right|$$
$$=$$

$$\begin{pmatrix} \frac{1}{2} & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{2} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{2} & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{2} \end{pmatrix}$$

The reduced density operators are obtained as

$$\hat{\rho}_{23} = Tr_1[\hat{\rho}_{123}] = \frac{1}{2}\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

and

$$\hat{\rho}_3 = Tr_{12}[\hat{\rho}_{123}] = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

which is equivalent to a completely un-polarized state,

12. Example-2 Another entangled GHZ state

The entangled GHZ state is given by

$$\left|\psi_{GHZ}{}^{(-)}\right\rangle = \frac{1}{\sqrt{2}}[\left|+++\right\rangle - \left|---\right\rangle]$$

The density operator is defined by

$$\hat{\rho}_{123} = \left|\psi_{GHZ}{}^{(-)}\right\rangle\left\langle\psi_{GHZ}{}^{(-)}\right| =$$

$$\begin{pmatrix} \frac{1}{2} & 0 & 0 & 0 & 0 & 0 & 0 & -\frac{1}{2} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -\frac{1}{2} & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{2} \end{pmatrix}$$

The reduced density operators are obtained as

$$\hat{\rho}_{23} = Tr_1[\hat{\rho}_{123}] = \frac{1}{2}\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

and

$$\hat{\rho}_3 = Tr_{12}[\rho_{123}]\frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

which is equivalent to a completely un-polarized state,

13. Origin of the collapse of the state vector

This is the origin of the collapse of the state vector. The collapse postulate states that upon the measurement a system evolves from pure state to mixed state.

i.e., if we are in a state $|\psi\rangle$ and we measure A, we end up in an eigenstate $|a\rangle$ with the probability $|\langle a|\psi\rangle|^2$.

i.e. the pure state $|\psi\rangle$ evolves to a mixed state

$$\hat{\rho} = \sum_a |\langle a|\psi\rangle|^2 |a\rangle\langle a|$$

where

$$\hat{A}|a\rangle = a|a\rangle .$$

This puzzle is resolved if we keep track of entanglements.

$|\psi\rangle$ = the state of system

$|E\rangle$ = the state of measuring apparatus

Measurement:

$$|a\rangle|E\rangle \to |a\rangle|E_a\rangle$$

where $|E_a\rangle$ is the state of apparatus after measuring $|a\rangle$.

If

$$|\psi\rangle = \sum_a \langle a|\psi\rangle|a\rangle$$

then by linearity measurement

$$|\psi\rangle|E\rangle \to \sum_a \langle a|\psi\rangle|a\rangle|E_a\rangle$$

If we do not wish to study the state of our apparatus, we must trace over H_E.

$$
\begin{aligned}
|\psi\rangle\langle\psi| \to & Tr_E[(\sum_a \langle a|\psi\rangle |a\rangle \otimes |E_a\rangle)(\sum_{a'} \langle\psi|a'\rangle\langle a'| \otimes \langle E_{a'}|) \\
&= Tr_E[\sum_{a,a'} \langle a|\psi\rangle\langle\psi|a'\rangle(|a\rangle \otimes |E_a\rangle)(\langle a'| \otimes \langle E_{a'}|) \\
&= Tr_E[\sum_{a,a'} \langle a|\psi\rangle\langle\psi|a'\rangle(|a\rangle\langle a'| \otimes (|E_a\rangle\langle E_{a'}|) \\
&= \sum_{a,a'} \langle a|\psi\rangle\langle\psi|a'\rangle(|a\rangle\langle a'|) Tr_E(|E_a\rangle\langle E_{a'}|) \\
&= \sum_{a,a'} \langle a|\psi\rangle\langle\psi|a'\rangle(|a\rangle\langle a'|)\delta_{a,a'} \\
&= \sum_{a'} |\langle a|\psi\rangle|^2 |a\rangle\langle a|
\end{aligned}
$$

where we use the formula

$$
\begin{aligned}
Tr_E(|a\rangle\langle a'| \otimes (|E_a\rangle\langle E_{a'}|) &= (|a\rangle\langle a'|) Tr_E(|E_a\rangle\langle E_{a'}|) \\
&= \langle E_{a'}|E_a\rangle(|a\rangle\langle a'|)
\end{aligned}
$$

The state vector is collapsed. They just get entangled. It is when we forgot about quantum density operator of measuring apparatus that they appears to collapse. Assume that $\langle E_a|E_{a'}\rangle = \delta_{a,a'}$, this is

$$
|\psi\rangle\langle\psi| \to \sum_a |\langle a|\psi\rangle|^2 |a\rangle\langle a|
$$

By choosing not to measure E we have reproduced the apparent collapse of the state vector in a unitary way.

The assumption that $\langle E_a|E_{a'}\rangle = \delta_{a,a'}$ is the statement that E is classical.
Why are some variable "classical" and some are not.

14. Schrodinger's cat

14.1 Bipartite quantum system

We consider the state vector in the $A \otimes B$ system. The system A is accessible, while the system B is inaccessible.

$$
|\psi\rangle_{AB} = a(|0\rangle_A \otimes |0\rangle_B) + b(|1\rangle_A \otimes |1\rangle_B) = \begin{pmatrix} a \\ 0 \\ 0 \\ b \end{pmatrix}
$$

where $\langle 0|0\rangle_A = \langle 1|1\rangle_A = 1$, $\langle 0|1\rangle_A = \langle 1|0\rangle_A = 0$, $\langle 0|0\rangle_B = \langle 1|1\rangle_B = 1$, $\langle 0|1\rangle_B = \langle 1|0\rangle_B = 0$, and

$$|a|^2 + |b|^2 = 1$$

Suppose that we measure the system A by projecting onto the $\{|0\rangle_A, |1\rangle_A\}$. With the probability $|a|^2$, we obtain the state $|0\rangle_A$. The state vector collapses into the state

$$|0\rangle_A \otimes |0\rangle_B .$$

With the probability $|b|^2$, we obtain the state $|1\rangle_A$. The state vector collapses into the state

$$1_A \otimes |1\rangle_B .$$

In either case, a definite state of the system B is picked out by the measurement. If we subsequently measure the system B, then we are guaranteed to find $|0\rangle_B$, and we are guaranteed to find $|1\rangle_B$, if we had found $|1\rangle_A$.

The density operator for the combined system AB is given by

$$\begin{aligned}
\hat{\rho}_{AB} &= |\psi\rangle_{AB}\langle\psi|_{AB} \\
&= [a|0\rangle_A \otimes |0\rangle_B + b|1\rangle_A \otimes |1\rangle_B][a^*\langle 0|_A \otimes \langle 0|_B + b^*\langle 1|_A \otimes \langle 1|_B] \\
&= |a|^2(|0\rangle_A\langle 0|_A \otimes |0\rangle_B\langle 0|_B) + |b|^2(|1\rangle_A\langle 1|_A \otimes |1\rangle_B\langle 1|_B) \\
&\quad + ab^*(|0\rangle_A\langle 1|_A \otimes |0\rangle_B\langle 1|_B) + a^*b(|1\rangle_A\langle 0|_A \otimes |1\rangle_B\langle 0|_B)]
\end{aligned}$$

The average value of the observable $\hat{M}_A \otimes \hat{1}_B$ in the state $|\psi\rangle_{AB}$ is

$$\begin{aligned}
\langle M_A\rangle &= \langle\psi_{AB}|\hat{M}_A \otimes \hat{1}_B|\psi_{AB}\rangle \\
&= [a^*(\langle 0|_A \otimes \langle 0|_B) + b^*(\langle 1|_A \otimes \langle 1|_B)] \\
&\quad \times [a(\hat{M}_A|0\rangle_A \otimes |0\rangle_B) + b(\hat{M}_A|1\rangle_A \otimes |1\rangle_B)] \\
&= |a|^2\langle 0|\hat{M}_A|0\rangle_A + |b|^2\langle 1|\hat{M}_A|1\rangle_A
\end{aligned}$$

since

$$(\hat{M}_A \otimes \hat{1}_B)|\psi\rangle_{AB} = a(\hat{M}_A|0\rangle_A \otimes |0\rangle_B) + b(\hat{M}_A|1\rangle_A \otimes |1\rangle_B)$$

$$\langle\psi_{AB}| = a^*(\langle 0|_A \otimes \langle 0|_B) + b^*(\langle 1|_A \otimes \langle 1|_B) = \begin{pmatrix} a^* \\ 0 \\ 0 \\ b^* \end{pmatrix}.$$

We introduce the density operator $\hat{\rho}_A$ of the system A (which is the reduced density operator), such that

$$\hat{\rho}_A = |a|^2 |0\rangle_A \langle 0|_A + |b|^2 |1\rangle_A \langle 1|_A$$

Then we have

$$\begin{aligned} Tr[\hat{M}_A \hat{\rho}_A] &= Tr[|a|^2 \hat{M}_A |0\rangle_A \langle 0|_A + |b|^2 \hat{M}_A |1\rangle_A \langle 1|_A] \\ &= |a|^2 \langle 0|\hat{M}_A|0\rangle_A + |b|^2 \langle 1|\hat{M}_A|1\rangle_A \\ &= \langle M_A \rangle \end{aligned}$$

So we have the expression

$$\langle M_A \rangle = Tr[\hat{M}_A \hat{\rho}_A]$$

Note that $\hat{\rho}_A$ represents an ensemble of possible quantum state, each occurring with a specified probability. $|a|^2$ is the probability in the state $|0\rangle_A$ and $|b|^2$ is the probability in the state $|1\rangle_A$.

14.2 Reduced operator

We show that $\hat{\rho}_A$ is the reduced density operator given by

$$\hat{\rho}_A = Tr_B[|\psi_{AB}\rangle\langle\psi_{AB}|].$$

In fact

$$\begin{aligned}
\hat{\rho}_A &= Tr_B[|a|^2(|0\rangle_A\langle 0|_A \otimes |0\rangle_B\langle 0|_B) + |b|^2(|1\rangle_A\langle 1|_A \otimes |1\rangle_B\langle 1|_B) \\
&\quad + ab^*(|0\rangle_A\langle 1|_A \otimes |0\rangle_B\langle 1|_B) + a^*b(|1\rangle_A\langle 0|_A \otimes |1\rangle_B\langle 0|_B)] \\
&= |a|^2(|0\rangle_A\langle 0|_A Tr_B[|0\rangle_B\langle 0|_B] + |b|^2|1\rangle_A\langle 1|_A Tr_B[|1\rangle_B\langle 1|_B] \\
&\quad + ab^*|0\rangle_A\langle 1|_A Tr_B[|0\rangle_B\langle 1|_B] + a^*b|1\rangle_A\langle 0|_A Tr_B[|1\rangle_B\langle 0|_B] \\
&= |a|^2|0\rangle_A\langle 0|_A\langle 0|0\rangle_B + |b|^2|1\rangle_A\langle 1|_A\langle 1|1\rangle_B \\
&\quad + ab^*|0\rangle_A\langle 1|_A\langle 0|1\rangle_B + a^*b|1\rangle_A\langle 0|_A\langle 1|0\rangle_B \\
&= |a|^2|0\rangle_A\langle 0|_A) + |b|^2(|1\rangle_A\langle 1|_A \\
&= \begin{pmatrix} |a|^2 & 0 \\ 0 & |b|^2 \end{pmatrix}
\end{aligned}$$

$\hat{\rho}_A$ for the subsystem A is obtained by performing a partial trace over subsystem B of the density operator for the combined system AB.

((**Another method**)) The matrix representation.

$$|\psi\rangle_{AB} = \begin{pmatrix} a \\ 0 \\ 0 \\ b \end{pmatrix}, \qquad \langle\psi_{AB}| = \begin{pmatrix} a^* & 0 & 0 & b^* \end{pmatrix}$$

$$|\psi_{AB}\rangle\langle\psi|_{AB} = \begin{pmatrix} a \\ 0 \\ 0 \\ b \end{pmatrix}\begin{pmatrix} a^* & 0 & 0 & b^* \end{pmatrix} = \begin{pmatrix} |a|^2 & 0 & 0 & ab^* \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ a^*b & 0 & 0 & |b|^2 \end{pmatrix}$$

$$\hat{\rho}_A = Tr_B[|\psi_{AB}\rangle\langle\psi_{AB}|] = \begin{pmatrix} |a|^2 & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & |b|^2 \end{pmatrix} = \begin{pmatrix} |a|^2 & 0 \\ 0 & |b|^2 \end{pmatrix}$$

Similarly, we have

$$\hat{\rho}_B = Tr_A[|\psi_{AB}\rangle\langle\psi_{AB}|] = \begin{pmatrix} |a|^2 & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & |b|^2 \end{pmatrix} = \begin{pmatrix} |a|^2 & 0 \\ 0 & |b|^2 \end{pmatrix}$$

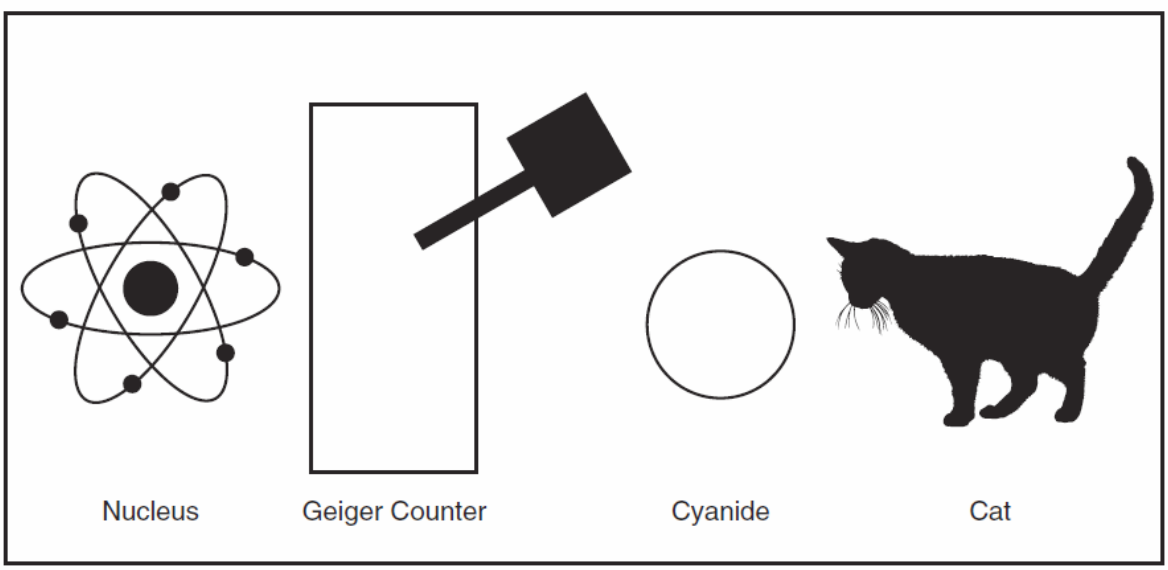
Then we have

$$\hat{\rho}_A = \hat{\rho}_B$$

The reduced density operator $\hat{\rho}_A$ contains the same information about the system A as the state vector of the combined system. We now understand how probabilities arise in quantum mechanics, when a quantum system A interacts with another system B. The systems A and B are entangled, that is correlated. The entanglement destroys the coherence of a superposition of states of A. so that some of the phase in the superposition becomes inaccessible if we look at A alone. We may describe this situation by saying that the state of system A collapses. It is in one of a set of alternative states, each of which can be assigned a probability.

14.3 Gedanken experiment Schrodinger's cat)

The Schrödinger cat paradox is a *gedanken* experiment designed by Schrödinger to illustrate some of the problems of quantum measurement, particularly in the extension of quantum mechanics to classical systems. The apparatus of Schrodinger's *gedanken* experiment consists of a radioactive nucleus, a Geiger counter, a hammer, a bottle of cyanide gas, a cat, and a box. The nucleus has a 50% probability of decaying in one hour. The components are assembled such that when the nucleus decays, it triggers the Geiger counter, which causes the hammer to break the bottle and release the poisonous gas, killing the cat. Thus, after one hour there is a 50% probability that the cat is dead.



((Schrödinger 1935))

> One can even set up quite ridiculous cases. A cat is penned up in a steel chamber, along with the following device (which must be secured against direct interference by the cat): in a Geiger counter there is a tiny bit of radioactive substance, so small, that perhaps in the course of the hour one of the atoms decays, but also, with equal probability, perhaps none;

if it happens, the counter tube discharges and through a relay releases a hammer which shatters a small flask of hydrocyanic acid. If one has left this entire system to itself for an hour, one would say that the cat still lives if meanwhile no atom has decayed. The psi-function of the entire system would express this by having in it the living and dead cat (pardon the expression) mixed or smeared out in equal parts. (E. Schrödinger, November 1935).

As an example of the usefulness of the density matrix, we consider Schrödinger's cat paradox. Schrödinger imagined placing a cat (the system A) in a box with some radioactive material. After one hour there is 50% probability that one of the radioactive atoms (the system B) decays, and this decay triggers a mechanism which kills the cat. Before the box is opened, and a measurement is performed to determine whether the cat is alive or dead. The apparatus is designed such that there is a one-to-one correspondence between the un-decayed nuclear state and the live-cat state and a one-to-one correspondence between the decayed nuclear state and the dead-cat state. Though the cat is macroscopic, it is made up of *microscopic particles* and so should be described by a quantum state, albeit a complicated one. Thus, we expect that the quantum state of the combined system AB after one hour is described

$$\begin{aligned}
|\psi_{AB}\rangle &= \frac{1}{\sqrt{2}}[|cat-alive\rangle_A \otimes |no-decay\rangle_B) + (|cat-dead\rangle_A \otimes |decay\rangle_B) \\
&= \frac{1}{\sqrt{2}}[|0\rangle_A \otimes |0\rangle_B) + (|1\rangle_A \otimes |1\rangle_B]
\end{aligned}$$

which is an entangled state, where

$$|cat-alive\rangle_A = |0\rangle_A, \qquad |cat-dead\rangle_A = |1\rangle_A$$

$$|no-decay\rangle_A = |0\rangle_B, \qquad |decay\rangle_A = |1\rangle_B$$

The density operator is given by

$$\begin{aligned}
\hat{\rho}_{AB} &= |\psi\rangle_{AB}\langle\psi|_{AB} \\
&= \frac{1}{2}[|0\rangle_A \otimes |0\rangle_B + |1\rangle_A \otimes |1\rangle_B][\langle 0|_A \otimes \langle 0|_B + \langle 1|_A \otimes \langle 1|_B] \\
&= \frac{1}{2}[|0\rangle_A\langle 0|_A \otimes |0\rangle_B\langle 0|_B + |1\rangle_A\langle 1|_A \otimes |1\rangle_B\langle 1|_B \\
&\quad + |0\rangle_A\langle 1|_A \otimes |0\rangle_B\langle 1|_B + |1\rangle_A\langle 0|_A \otimes |1\rangle_B\langle 0|_B]
\end{aligned}$$

or, using the matrix representation,

$$\hat{\rho}_{AB} = \frac{1}{2}\begin{pmatrix}1\\0\\0\\1\end{pmatrix}\begin{pmatrix}1 & 0 & 0 & 1\end{pmatrix} = \frac{1}{2}\begin{pmatrix}1 & 0 & 0 & 1\\0 & 0 & 0 & 0\\0 & 0 & 0 & 0\\1 & 0 & 0 & 1\end{pmatrix}$$

The reduced density operator $\hat{\rho}_A$ for the system A is

$$\begin{aligned}\hat{\rho}_A &= Tr_B[|\psi_{AB}\rangle\langle\psi_{AB}|]\\ &= \frac{1}{2}(|0\rangle_A\langle 0|_A + |1\rangle_A\langle 1|_A)\\ &= \frac{1}{2}\begin{pmatrix}1 & 0\\0 & 1\end{pmatrix}\end{aligned}$$

where

$$\begin{aligned}Tr_B[|\psi_{AB}\rangle\langle\psi_{AB}|] &= \frac{1}{2}Tr_B[(|0\rangle_A\langle 0|_A \otimes |0\rangle_B\langle 0|_B) + (|1\rangle_A\langle 1|_A \otimes |1\rangle_B\langle 1|_B)\\ &\quad + (|0\rangle_A \otimes |0\rangle_B \otimes \langle 1|_A \otimes \langle 1|_B) + (|1\rangle_A \otimes |1\rangle_B \otimes \langle 0|_A \otimes \langle 0|_B])]\\ &= \frac{1}{2}|0\rangle_B\langle 0|_B Tr_A[|0\rangle_A\langle 0|_A] + \frac{1}{2}|1\rangle_B\langle 1|_B Tr_A[|1\rangle_A\langle 1|_A]\\ &= \frac{1}{2}|0\rangle_B\langle 0|_B\langle 0|0\rangle_A + \frac{1}{2}|1\rangle_B\langle 1|_B\langle 1|1\rangle_A\\ &= \frac{1}{2}|0\rangle_B\langle 0|_B + \frac{1}{2}|1\rangle_B\langle 1|_B\\ &= \frac{1}{2}\begin{pmatrix}1 & 0\\0 & 1\end{pmatrix}\end{aligned}$$

Using the formula,

$$\begin{aligned}\langle M_A\rangle &= Tr[\hat{M}_A\hat{\rho}_A]\\ &= \frac{1}{2}[\langle 0|\hat{M}_A|0\rangle_A + \langle 1|\hat{M}_A|1\rangle_A]\end{aligned}$$

We can calculate the probability

(a) $\hat{M}_A = |0\rangle\langle 0|_A$

$$Tr[\hat{M}_A\hat{\rho}_A]=\frac{1}{2}]$$

(b) $\hat{M}_A=|1\rangle\langle 1|_A$

$$Tr[\hat{M}_A\hat{\rho}_A]=\frac{1}{2}$$

$\hat{\rho}_A$ represents an ensemble of possible quantum state for the system A (corresponding to the in-polarized state for the photon system), each occurring with a specified probability. $\frac{1}{2}$ is the probability in the state $|0=cat-alive\rangle_A$ and $\frac{1}{2}$ is the probability in the state $|1=cat-dead\rangle_A$.

The reduced density operator $\hat{\rho}_A$ for the system A is

$$\begin{aligned}\hat{\rho}_B &= Tr_A[|\psi_{AB}\rangle\langle\psi_{AB}|] \\ &= \frac{1}{2}(|0\rangle_B\langle 0|_B+|1\rangle_B\langle 1|_B) \\ &= \frac{1}{2}\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}\end{aligned}$$

$\hat{\rho}_A$ represents an ensemble of possible quantum state for the system B, each occurring with a specified probability. $\frac{1}{2}$ is the probability in the state $|0=non-decay\rangle_B$ and $\frac{1}{2}$ is the probability in the state $|1=cat-dead\rangle_B$.

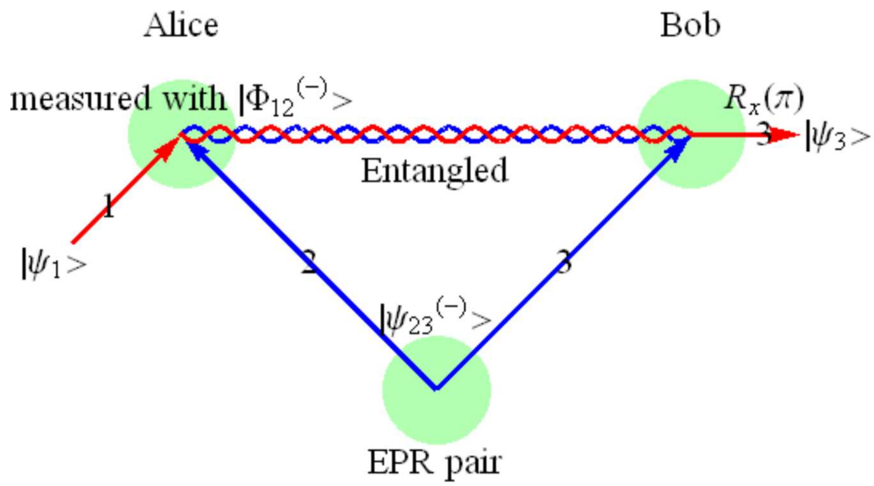
((**Note**)) **Maximally entangled state**

Maximally entangled state means that when we trace over the system B to find the density operator $\hat{\rho}_A$ of the system B, we obtain a multiple of the identity operator

$$\hat{\rho}_A=\frac{1}{2}\hat{1}_A$$

(and similarly, $\hat{\rho}_B=\frac{1}{2}\hat{1}_B$). This means that if we measure spin A along any axis, the result is completely random. We find spin up with probability 1/2 and spin down with probability 1/2.

15. Quantum teleportation



We consider the pure particle state $\left|\psi_{123}\right\rangle$ which is related to the quantum teleportation. The density operator for this pure state is given by

$$\hat{\rho}_{123} = \left|\psi_{123}\right\rangle\left\langle\psi_{123}\right|$$

where

$$\left|\psi_{123}\right\rangle = \frac{1}{2}\left|\psi_{12}^{(-)}\right\rangle[-a\left|+z\right\rangle_3 - b\left|-z\right\rangle_3] + \frac{1}{2}\left|\psi_{12}^{(+)}\right\rangle[-a\left|+z\right\rangle_3 + b\left|-z\right\rangle_3]$$
$$+ \frac{1}{2}\left|\Phi_{12}^{(-)}\right\rangle[a\left|-z\right\rangle_3 + b\left|+z\right\rangle_3] + \frac{1}{2}\left|\Phi_{12}^{(+)}\right\rangle[a(\left|-z\right\rangle_3 - b\left|+z\right\rangle_3)$$

with

$$\left|\psi_{12}^{(\pm)}\right\rangle = \frac{1}{\sqrt{2}}[\left|+z\right\rangle_1\left|-z\right\rangle_2 \pm \left|-z\right\rangle_1\left|+z\right\rangle_2] = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \\ \pm 1 \\ 0 \end{pmatrix}$$

$$\left|\Phi_{12}^{(\pm)}\right\rangle = \frac{1}{\sqrt{2}}[\left|+z\right\rangle_1\left|+z\right\rangle_2 \pm \left|-z\right\rangle_1\left|-z\right\rangle_2] = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ 0 \\ \pm 1 \end{pmatrix}.$$

Note that

$$|a|^2 + |b|^2 = 1.$$

The density operator $\hat{\rho}_{123}$ can be obtained as

$$\hat{\rho}_{123} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & |a|^2/2 & -|a|^2/2 & 0 & 0 & (ab^*)/2 & -(ab^*)/2 & 0 \\ 0 & -|a|^2/2 & |a|^2/2 & 0 & 0 & -(ab^*)/2 & (ab^*)/2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & (a^*b)/2 & -(a^*b)/2 & 0 & 0 & |b|^2/2 & -|b|^2/2 & 0 \\ 0 & -(a^*b)/2 & (a^*b)/2 & 0 & 0 & -|b|^2/2 & |b|^2/2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

Tracing out particle 1, the reduced density operators are obtained as

$$\begin{aligned} \hat{\rho}_{23} &= Tr_1[\hat{\rho}_{123}] \\ &= \frac{1}{2}\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & |a|^2 & -|a|^2 & 0 \\ 0 & -|a|^2 & |a|^2 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} + \frac{1}{2}\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & |b|^2 & -|b|^2 & 0 \\ 0 & -|b|^2 & |b|^2 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \\ &= \frac{1}{2}\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & |a|^2+|b|^2 & -|a|^2-|b|^2 & 0 \\ 0 & -|a|^2-|b|^2 & |a|^2+|b|^2 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \\ &= \frac{1}{2}\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \end{aligned}$$

Tracing over particle 2 furthermore, we have

$$\hat{\rho}_3 = Tr_{12}[\hat{\rho}_{123}] = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + \frac{1}{2}\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

which is equivalent to a completely un-polarized state. So Bob (particle 3) has no information about the state of the particle Alice is attempting to teleport. On the other hand, if Bob waits until he receives the result of Alice's Bell state measurement, Bob can then maneuver his particle into the state $|\psi\rangle$ that Alice's particle was in initially.

((**Mathematica**))

```
Clear["Global`*"];
exp_* := exp /. {Complex[re_, im_] :> Complex[re, -im]};
ψ1 = 1/√2 {{0}, {1}, {-1}, {0}}; ψ2 = 1/√2 {{0}, {1}, {1}, {0}};
ϕ1 = 1/√2 {{1}, {0}, {0}, {-1}};
ϕ2 = 1/√2 {{1}, {0}, {0}, {1}};
χ1 = {{-a}, {-b}}; χ2 = {{-a}, {b}}; χ3 = {{b}, {a}}; χ4 = {{-b}, {a}};
ψ123 = 1/2 KroneckerProduct[ψ1, χ1] + 1/2 KroneckerProduct[ψ2, χ2] +
    1/2 KroneckerProduct[ϕ1, χ3] + 1/2 KroneckerProduct[ϕ2, χ4] //
   Simplify;
K1 = ψ123;
K2 = Transpose[ψ123] //. {a → a1, b → b1};
ρ = K1.K2 // FullSimplify; ρ // MatrixForm
```

$$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{a\,a1}{2} & -\frac{a\,a1}{2} & 0 & 0 & \frac{a\,b1}{2} & -\frac{a\,b1}{2} & 0 \\ 0 & -\frac{a\,a1}{2} & \frac{a\,a1}{2} & 0 & 0 & -\frac{a\,b1}{2} & \frac{a\,b1}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{a1\,b}{2} & -\frac{a1\,b}{2} & 0 & 0 & \frac{b\,b1}{2} & -\frac{b\,b1}{2} & 0 \\ 0 & -\frac{a1\,b}{2} & \frac{a1\,b}{2} & 0 & 0 & -\frac{b\,b1}{2} & \frac{b\,b1}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

16. Average $\langle \hat{X}_1 \rangle$

We consider the average value of an operator $\hat{X}_1$ that acts only on the system 1 in a global density operator $\hat{\rho}$ for the particles 1 and 2;

$$\langle \hat{X}_1 \rangle = Tr_{12}[(\hat{X}_1 \otimes \hat{I}_2)\hat{\rho}_{12}] = Tr_1[\hat{X}_1 Tr_2 \hat{\rho}_{12}] = Tr_1[\hat{X}_1 \hat{\rho}_1]$$

where

$$\hat{\rho}_1 = Tr_2 \hat{\rho}$$

Since $\hat{\rho}_{12} = \hat{\rho}_1 \otimes \hat{\rho}_2$, we have

$$\begin{aligned} \langle \hat{X}_1 \rangle &= Tr[(\hat{X}_1 \otimes \hat{I}_2)\hat{\rho}_{12}] \\ &= Tr[(\hat{X}_1 \otimes \hat{I}_2)(\hat{\rho}_1 \otimes \hat{\rho}_2)] \\ &= Tr[(\hat{X}_1 \hat{\rho}_1 \otimes \hat{I}_2 \hat{\rho}_2)] \\ &= Tr_1[\hat{X}_1 \hat{\rho}_1] Tr[\hat{I}_2 \hat{\rho}_2] \\ &= Tr_1[\hat{X}_1 \hat{\rho}_1] \end{aligned}$$

and

$$\hat{\rho}_1 = Tr_2[\hat{\rho}_1 \otimes \hat{\rho}_2] = \hat{\rho}_1 Tr_2[\hat{\rho}_2] = \hat{\rho}_1$$

17. Schmidt decomposition

((**Theorem**))

Suppose that $|\psi\rangle$ is a pure state of a biparticle composite system, $A \otimes B$. Then there exist orthonormal states $|i_A\rangle$ for system *A*, and $|i_B\rangle$ for system, *B* such that

$$|\psi\rangle = \sum_i \sqrt{p_i}|i_A\rangle|i_B\rangle,$$

where $\lambda_i = \sqrt{p_i}$ is known as Schmidt coefficient and is non-negative real number satisfying

$$\sum_i \lambda_i^2 = 1, \qquad \text{or} \qquad \sum_i p_i = 1$$

The states $|i_A\rangle$ and $|i_B\rangle$ are any fixed orthonormal bases for *A* and *B* (the relevant state spaces are here of the same dimension).

The density operator is defined by

$$\hat{\rho} = |\psi\rangle\langle\psi|.$$

Note that

$$Tr[\hat{\rho}^2] = \sum_i \lambda_i^2.$$

If $Tr[\hat{\rho}^2] = 1$ (pure state), $\lambda_i = 1$ for one and only one *i* and zero for all others

---

We consider the simple case.

$$|\psi\rangle = C_{11}|a_1\rangle|b_1\rangle + C_{12}|a_1\rangle|b_2\rangle + C_{21}|a_2\rangle|b_1\rangle + C_{22}|a_2\rangle|b_1\rangle$$

$$|\psi\rangle = \sqrt{p_1}|v_1\rangle|w_1\rangle + \sqrt{p_2}|v_2\rangle|w_2\rangle$$

where $p_1 + p_2 = 1$.

The unitary transformation:

$$|v_1\rangle = \hat{U}|a_1\rangle = U_{11}|a_1\rangle + U_{21}|a_2\rangle$$

$$|v_2\rangle = \hat{U}|a_2\rangle = U_{12}|a_1\rangle + U_{22}|a_2\rangle$$

where

$$\hat{U} = \begin{pmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{pmatrix}, \qquad \hat{U}^{+}\hat{U} = \hat{1}$$

We also have

$$|w_1\rangle = \hat{V}|b_1\rangle = V_{11}|b_1\rangle + V_{21}|b_2\rangle$$

$$|w_2\rangle = \hat{V}|b_2\rangle = V_{12}|b_1\rangle + V_{22}|b_2\rangle$$

where

$$\hat{V} = \begin{pmatrix} V_{11} & V_{12} \\ V_{21} & V_{22} \end{pmatrix}, \qquad \hat{V}^{+}\hat{V} = \hat{1}$$

Then

$$\begin{aligned}
|\psi\rangle &= \sqrt{p_1}|v_1\rangle|w_1\rangle + \sqrt{p_2}|v_2\rangle|w_2\rangle \\
&= \sqrt{p_1}(U_{11}|a_1\rangle + U_{21}|a_2\rangle(V_{11}|b_1\rangle + V_{21}|b_2\rangle) \\
&\quad + \sqrt{p_2}(U_{12}|a_1\rangle + U_{22}|a_2\rangle(V_{12}|b_1\rangle + V_{22}|b_2\rangle) \\
&= (\sqrt{p_1}U_{11}V_{11} + \sqrt{p_2}U_{12}V_{12})|a_1\rangle|b_1\rangle + (\sqrt{p_1}U_{11}V_{21} + \sqrt{p_2}U_{12}V_{22})|a_1\rangle|b_2\rangle \\
&\quad + (\sqrt{p_1}U_{21}V_{11} + \sqrt{p_2}U_{22}V_{12})|a_2\rangle|b_1\rangle + (\sqrt{p_1}U_{21}V_{21} + \sqrt{p_2}U_{22}V_{22})|a_2\rangle|b_2\rangle
\end{aligned}$$

Then we have

$$C_{11} = U_{11}\sqrt{p_1}V_{11} + U_{12}\sqrt{p_2}V_{12}, \qquad C_{12} = U_{11}\sqrt{p_1}V_{21} + U_{12}\sqrt{p_2}V_{22}$$

$$C_{21} = U_{21}\sqrt{p_1}V_{11} + U_{22}\sqrt{p_2}V_{12} \qquad C_{22} = U_{21}\sqrt{p_1}V_{21} + U_{22}\sqrt{p_2}V_{22}$$

Using the matrix form, we get

$$\begin{aligned}\hat{C} &= \begin{pmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{pmatrix}\begin{pmatrix} \sqrt{p_1} & 0 \\ 0 & \sqrt{p_2} \end{pmatrix}\begin{pmatrix} V_{11} & V_{21} \\ V_{12} & V_{22} \end{pmatrix} \\ &= \begin{pmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{pmatrix}\begin{pmatrix} \sqrt{p_1} & 0 \\ 0 & \sqrt{p_2} \end{pmatrix}\begin{pmatrix} V_{11} & V_{12} \\ V_{21} & V_{22} \end{pmatrix}^T \\ &= \hat{U}\hat{d}\hat{V}^T\end{aligned}$$

Under the basis of $\{\left|a_i, b_j\right\rangle = \left|a_i\right\rangle \otimes \left|b_{ji}\right\rangle$, where $\hat{d}$ is a non-negative diagonal matrix, and $\hat{V}^T$ is the transpose matrix of $\hat{V}$.

$$\hat{d} = \begin{pmatrix} \sqrt{p_1} & 0 \\ 0 & \sqrt{p_2} \end{pmatrix}$$

Thus we have

$$\begin{aligned}\hat{C}\hat{C}^+ &= (\hat{U}\hat{d}\hat{V}^T)(\hat{U}\hat{d}\hat{V}^T)^+ \\ &= (\hat{U}\hat{d}\hat{V}^T)(\hat{V}^{+T}\hat{d}^+\hat{U}^+) \\ &= \hat{U}\hat{d}\hat{d}^+\hat{U}^+\end{aligned}$$

$$\begin{aligned}\hat{U}^+(\hat{C}\hat{C}^+)\hat{U} &= \hat{d}\hat{d}^+ \\ &= \begin{pmatrix} p_1 & 0 \\ 0 & p_2 \end{pmatrix}\end{aligned}$$

In order to determine the values of p_1 and p_2, we need to solve the eigenvalue problem of $\hat{C}\hat{C}^+$, if $\hat{C}\hat{C}^+$ is not a diagonal matrix.

Thus we can calculate the Schmidt numbers

Schmidt decomposition

$$(\hat{A} \otimes \hat{B})(\hat{C} \otimes \hat{D}) = (\hat{A}\hat{C}) \otimes (\hat{B}\hat{D})$$

$$(\hat{A} \otimes \hat{B})^+ = \hat{A}^+ \otimes \hat{B}^+$$

$$(\hat{A}\otimes\hat{B})^T = \hat{A}^T \otimes \hat{B}^T$$

$$(\hat{A}\otimes\hat{B})^{-1} = \hat{A}^{-1} \otimes \hat{B}^{-1}$$

$$\begin{aligned}\left|v_i\right\rangle \otimes \left|w_j\right\rangle &= (\hat{U}\left|a_i\right\rangle) \otimes (\hat{V}\left|b_j\right\rangle) \\ &= (\hat{U}\otimes\hat{V})(\left|a_i\right\rangle \otimes \left|b_j\right\rangle)\end{aligned}$$

Eigenvalue problem

$$\hat{C}(\left|v_i\right\rangle \otimes \left|w_j\right\rangle) = \sqrt{p_i}\delta_{i,j}(\left|v_i\right\rangle \otimes \left|w_j\right\rangle)$$

or

$$\hat{C}(\hat{U}\otimes\hat{V})(\left|a_i\right\rangle \otimes \left|b_j\right\rangle) = \sqrt{p_i}\delta_{i,j}(\hat{U}\otimes\hat{V})(\left|a_i\right\rangle \otimes \left|b_i\right\rangle)$$

or

$$\begin{aligned}\hat{C}^+\hat{C}(\hat{U}\otimes\hat{V})(\left|a_i\right\rangle \otimes \left|b_j\right\rangle) &= \sqrt{p_i}\delta_{i,j}\hat{C}^+(\hat{U}\otimes\hat{V})(\left|a_i\right\rangle \otimes \left|b_j\right\rangle) \\ &= p_i\delta_{i,j}(\hat{U}\otimes\hat{V})(\left|a_i\right\rangle \otimes \left|b_j\right\rangle)\end{aligned} \qquad (1)$$

where $\delta_{i,j}$ is the Kronecker delta. Here we note that

$$(\hat{U}\otimes\hat{V})^+ = \hat{U}^+ \otimes \hat{V}^+$$

$$\begin{aligned}(\hat{U}\otimes\hat{V})^+(\hat{U}\otimes\hat{V}) &= (\hat{U}^+\otimes\hat{V}^+)(\hat{U}\otimes\hat{V}) \\ &= (\hat{U}^+\hat{U})\otimes(\hat{V}^+\hat{V}) \\ &= \hat{1}\otimes\hat{1}\end{aligned}$$

Thus, Eq.(1) can be rewritten as

$$(\hat{U}\otimes\hat{V})^+\hat{C}^+\hat{C}(\hat{U}\otimes\hat{V})(\left|a_i\right\rangle \otimes \left|b_j\right\rangle) = p_i\delta_{i,j}\left|a_i\right\rangle \otimes \left|b_j\right\rangle \qquad (2)$$

When we introduce a new unitary operator,

$$\hat{X}(u,v) = \hat{U} \otimes \hat{V}$$

we get

$$X^{+}(u,v)\hat{C}^{+}\hat{C}X(u,v)(|a_i\rangle \otimes |b_j\rangle) = p_i\delta_{i,j}\,|a_i\rangle \otimes |b_j\rangle$$

or

$$\hat{C}^{+}\hat{C}X(u,v)(|a_i\rangle \otimes |b_j\rangle) = p_i\delta_{i,j}X(u,v)|a_i\rangle \otimes |b_j\rangle$$

under the basis of $\{|a_i\rangle \otimes |b_j\rangle\}$. So, we need to solve the eigenvalue problem of matrix $\hat{C}^{+}\hat{C}$ under the basis of $|a_i\rangle \otimes |b_j\rangle$ to determine the eigenvalue p_i.

((**Example-1**)) Pure state

$$|\psi\rangle = \frac{1}{\sqrt{2}}[|00\rangle + |01\rangle]$$

We construct $\hat{C}$ and $\hat{C}^{+}\hat{C}$.

$$\hat{C} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 0 & 0 \end{pmatrix}, \qquad \hat{C}^{+}\hat{C} = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$$

The eigenvlaue problem of $\hat{C}^{+}\hat{C}$;

eigenvalue; $p_1 = 1$, eigenket: $\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$.

eigenvalue; $p_2 = 0$, eigenket: $\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$.

So, there is only one nonzero Schmidt coefficient and thus $|\psi\rangle$ is a product state.

((**Example-2**)) Entangled state

$$|\psi\rangle = \frac{1}{\sqrt{2}}[|00\rangle + |11\rangle]$$

We construct $\hat{C}$ and $\hat{C}^{+}\hat{C}$.

$$\hat{C} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \qquad \hat{C}^{+}\hat{C} = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

The eigenvlaue problem of $\hat{C}^{+}\hat{C}$;

eigenvalue; $p_1 = \frac{1}{2}$, eigenket: $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$.

eigenvalue; $p_2 = \frac{1}{2}$, eigenket: $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$.

So there are two nonzero Schmidt coefficients and thus $|\psi\rangle$ is an entangled state.

((**Example-3**)) Entangled state

$$|\psi\rangle = \frac{1}{\sqrt{2}}[|01\rangle + |10\rangle]$$

We construct $\hat{C}$ and $\hat{C}^{+}\hat{C}$.

$$\hat{C} = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \hat{C}^{+}\hat{C} = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

The eigenvlaue problem of $\hat{C}^{+}\hat{C}$;

eigenvalue; $p_1 = \frac{1}{2}$, eigenket: $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$.

eigenvalue; $p_2 = \frac{1}{2}$, eigenket: $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$.

So there are two nonzero Schmidt coefficients and thus $|\psi\rangle$ is an entangled state

((**Example-4**))

$$|\psi\rangle = \frac{1}{\sqrt{3}}[|00\rangle + |01\rangle + |11\rangle]$$

We construct $\hat{C}$ and $\hat{C}^{+}\hat{C}$.

$$\hat{C} = \frac{1}{\sqrt{3}}\begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}, \qquad \hat{C}^{+}\hat{C} = \frac{1}{3}\begin{pmatrix} 1 & 1 \\ 1 & 2 \end{pmatrix}$$

The eigenvlaue problem of $\hat{C}^{+}\hat{C}$;

eigenvalue; $p_1 = 0.873$, eigenket: $\begin{pmatrix} 0.53 \\ 0.85 \end{pmatrix}$.

eigenvalue; $p_2 = 0.127$, eigenket: $\begin{pmatrix} 0.85 \\ -0.53 \end{pmatrix}$.

So there are two nonzero Schmidt coefficients and thus $|\psi\rangle$ is an entangled state.

((**Example-5**))

$$|\psi\rangle = \frac{1}{2}[|00\rangle - |01\rangle - |10\rangle + |11\rangle] = 1[\frac{1}{\sqrt{2}}|0\rangle - \frac{1}{\sqrt{2}}|1\rangle][\frac{1}{\sqrt{2}}|0\rangle - \frac{1}{\sqrt{2}}|1\rangle]$$

We construct $\hat{C}$ and $\hat{C}^{+}\hat{C}$.

$$\hat{C} = \frac{1}{2}\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}, \qquad \hat{C}^{+}\hat{C} = \frac{1}{2}\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}$$

The eigenvlaue problem of $\hat{C}^{+}\hat{C}$;

eigenvalue; $p_1 = 1$, eigenket: $\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$.

eigenvalue; $p_2 = 0$, eigenket: $\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$.

So there are one nonzero Schmidt coefficients and thus $|\psi\rangle$ is a product state.

((**Example-6**))

$$|\psi\rangle = \frac{1}{2\sqrt{6}}[(1+\sqrt{6})|00\rangle + (1-\sqrt{6})|01\rangle + (\sqrt{2}-\sqrt{3})|10\rangle + (\sqrt{2}+\sqrt{3})|11\rangle]$$

We construct $\hat{C}$ and $\hat{C}^{+}\hat{C}$.

$$\hat{C} = \frac{1}{2\sqrt{6}}\begin{pmatrix} 1+\sqrt{6} & 1-\sqrt{6} \\ \sqrt{2}-\sqrt{3} & \sqrt{2}+\sqrt{3} \end{pmatrix}, \qquad \hat{C}^{+}\hat{C} = \frac{1}{4}\begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix}$$

The eigenvlaue problem of $\hat{C}^{+}\hat{C}$;

eigenvalue; $p_1 = \frac{1}{4}$, eigenket: $\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$.

eigenvalue; $p_2 = \frac{3}{4}$, eigenket: $\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$.

So there are one nonzero Schmidt coefficients and thus $|\psi\rangle$ is an entangled state.

18. Schmidt decomposition application

It is very easy to compute the reduced density operator given the Schmidt decomposition

$$|\psi\rangle = \sum_i \sqrt{p_i}|i_A\rangle|i_B\rangle$$

The density operator is

$$\hat{\rho} = \sum_{i,j} \sqrt{p_i p_j}|i_A\rangle|i_B\rangle\langle j_A|\langle j_B|$$

The reduced density operator is given by

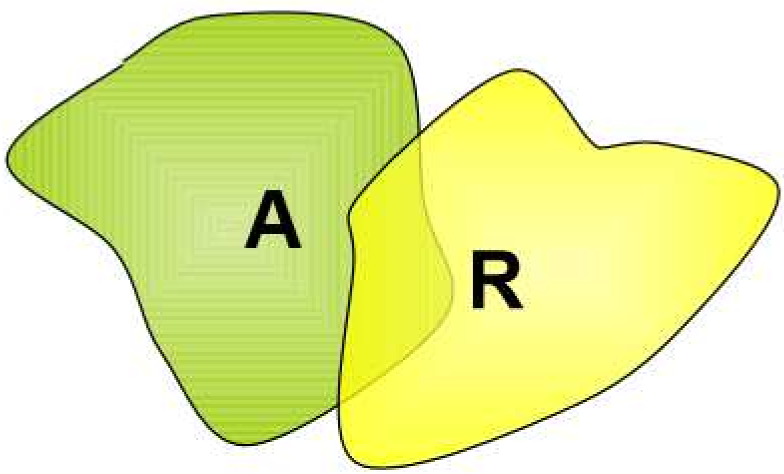
$$Tr_B(\hat{\rho}) = \sum_{i,j,k} \sqrt{p_i p_j} \langle k_B | i_B \rangle \langle j_B | k_B \rangle | i_A \rangle \langle j_A |$$
$$= \sum_i p_i | i_A \rangle \langle i_A |$$

$$Tr_A(\hat{\rho}) = \sum_{i,j,k} \sqrt{p_i p_j} \langle k_A | i_A \rangle \langle j_A | k_A \rangle | i_B \rangle \langle j_B |$$
$$= \sum_i p_i | i_B \rangle \langle i_B |$$

We note that the spectrum (i.e., set of eigenvalues) of both reduced density operators are the same.

19. Purification

Suppose we are given a state $\hat{\rho}_A$ of a quantum system *A*. It is possible to introduce an additional system, which we denote *R* (*R* has the same dimension as *A*) and define a pure state $|AR\rangle$ for the joint system *AR*



such that

$$\hat{\rho}_A = Tr_R |AR\rangle\langle AR|.$$

That is, the pure state $|AR\rangle$ reduces to $\hat{\rho}_A$ when we look at system *A* alone. This is a purely mathematical procedure, known as *purification*, which allows us to associate pure states with mixed states. For this reason we call system *R* a reference system: it is a fictitious system, without a direct physical significance.

((**Proof**))

To prove that purification can be done for *any* state, we explain how to construct a system *R* and purification $|AR\rangle$ for $\hat{\rho}_A$. Suppose $\hat{\rho}_A$ has orthonormal decomposition

$$\hat{\rho}_A = \sum_i p_i |i_A\rangle\langle i_A| \qquad \text{(mixed state)}$$

To purify $\hat{\rho}_A$, we introduce an additional system *R* which has the same dimension as system *A*, with orthonormal basis states $|i_R\rangle$, and define a pure state for the combined system

$$|AR\rangle = \sum_i \sqrt{p_i} |i_A\rangle |i_R\rangle \qquad \text{(pure state)}$$

We now calculate the reduced density operator for the system *A* corresponding to the state $|AR\rangle$

$$\begin{aligned}
Tr_R(|AR\rangle\langle AR|) &= \sum_{i,j} \sqrt{p_i}\sqrt{p_j}\, Tr(|i_A\rangle|i_R\rangle\langle j_A|\langle j_R|) \\
&= \sum_{i,j} \sqrt{p_i}\sqrt{p_j}\, |i_A\rangle\langle j_A| Tr(|i_R\rangle\langle j_R|) \\
&= \sum_{i,j} \sqrt{p_i}\sqrt{p_j}\, |i_A\rangle\langle j_A| \delta_{ij} \\
&= \sum_{i,j} p_i |i_A\rangle\langle i_A| \\
&= \hat{\rho}_A
\end{aligned}$$

Thus $|AR\rangle$ is a purification of $\hat{\rho}_A$.

Notice the close relationship of the Schmidt decomposition to purification: the procedure used to purify a mixed state of system *A* is to define a pure state whose Schmidt basis for system *A* is just the basis in which the mixed state is diagonal, with the Schmidt coefficients being the square root of the eigenvalues of the density operator being purified.

20. ((Example-1))

Given the density operator

$$\hat{\rho} = \frac{1}{2}[|+z\rangle\langle +z| + |-z\rangle\langle -z| - |-z\rangle\langle +z| - |+z\rangle\langle -z|] = \frac{1}{2}\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix},$$

construct the density matrix. Use the density operator formalism to calculate $\langle S_x \rangle$ for this state. Is this the density operator for a pure state? Justify your answer in two different ways.

((**Solution**))

$$\hat{\rho} = \frac{1}{2}\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}$$

$$Tr[\hat{\rho}^2] = Tr[\hat{\rho}] = 1 \qquad \text{(pure state)}$$

$$Tr[\hat{\rho}\hat{S}_x] = -\frac{\hbar}{2}$$

((**Mathematica**))

```
Clear["Global`*"]; Sx = ħ/2 (0 1
                             1 0);
ρ =
 1/2 (Outer[Times, {1, 0}, {1, 0}] +
    Outer[Times, {0, 1}, {0, 1}] -
    Outer[Times, {0, 1}, {1, 0}] -
    Outer[Times, {1, 0}, {0, 1}])
{{1/2, -1/2}, {-1/2, 1/2}}

Tr[Sx.ρ]
-ħ/2

ρ.ρ - ρ // Simplify
{{0, 0}, {0, 0}}
```

---

21. ((Example-2))

Show that

$$\hat{\rho} = \frac{1}{2}[|+\boldsymbol{n}\rangle\langle+\boldsymbol{n}| + |-\boldsymbol{n}\rangle\langle-\boldsymbol{n}|] = \frac{1}{2}[|+z\rangle\langle+z| + |-z\rangle\langle-z|]$$

where

$$|+\boldsymbol{n}\rangle = \begin{pmatrix} \cos\frac{\theta}{2} \\ e^{i\phi}\sin\frac{\theta}{2} \end{pmatrix}, \qquad |-\boldsymbol{n}\rangle = \begin{pmatrix} \sin\frac{\theta}{2} \\ -e^{i\phi}\cos\frac{\theta}{2} \end{pmatrix}$$

((**Solution**))

$$\hat{\rho}_z = \frac{1}{2}[|+z\rangle\langle+z| + |-z\rangle\langle-z|] = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$\hat{\rho}_{\boldsymbol{n}} = \frac{1}{2}[|+\boldsymbol{n}\rangle\langle+\boldsymbol{n}| + |-\boldsymbol{n}\rangle\langle-\boldsymbol{n}|] = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

Then we have

$$\hat{\rho}_{\boldsymbol{n}} = \hat{\rho}_z$$

$$Tr[\hat{\rho}^2] = \frac{1}{2} \qquad \text{(for mixed state)}$$

((**Mathematica**))

```
Clear["Global`*"];
expr_* := expr /. Complex[a_, b_] :> Complex[a, -b];
ψpn = {Cos[θ/2], Exp[ⅈ ϕ] Sin[θ/2]};
ψmn = {Sin[θ/2], -Exp[ⅈ ϕ] Cos[θ/2]};
ρ =
 1/2 Outer[Times, ψpn, ψpn*] +
   1/2 Outer[Times, ψmn, ψmn*] // Simplify
```

$\{\{\frac{1}{2}, 0\}, \{0, \frac{1}{2}\}\}$

```
Tr[ρ.ρ]
```

$\frac{1}{2}$

---

22. ((Example-3))

Find states $|\psi_1\rangle$ and $|\psi_1\rangle$ for which the density operator

$$\hat{\rho} = \frac{3}{4}|+z\rangle\langle +z| + \frac{1}{4}|-z\rangle\langle -z|$$

can be expressed in the form

$$\hat{\rho} = \frac{1}{2}|\psi_1\rangle\langle\psi_1| + \frac{1}{2}|\psi_2\rangle\langle\psi_2|$$

((**Solution**))

Assume that

$$|\psi_1\rangle = \frac{\sqrt{3}}{2}|+z\rangle + \frac{1}{2}|-z\rangle = \begin{pmatrix} \frac{\sqrt{3}}{2} \\ \frac{1}{2} \end{pmatrix}$$

$$|\psi_2\rangle = \frac{\sqrt{3}}{2}|+z\rangle - \frac{1}{2}|-z\rangle = \begin{pmatrix} \frac{\sqrt{3}}{2} \\ -\frac{1}{2} \end{pmatrix}.$$

Then we have

$$\hat{\rho} = \frac{1}{2}|\psi_1\rangle\langle\psi_1| + \frac{1}{2}|\psi_2\rangle\langle\psi_2| = \frac{3}{4}|+z\rangle\langle+z| + \frac{1}{4}|-z\rangle\langle-z| = \begin{pmatrix} \frac{3}{4} & 0 \\ 0 & \frac{1}{4} \end{pmatrix}.$$

with

$$Tr[\hat{\rho}^2] = \frac{5}{8}$$

((**Mathematica**))

```
Clear["Global`*"];
expr_* := expr /. Complex[a_, b_] :> Complex[a, -b];
ψ1 = {√3/2, 1/2}; ψ2 = {√3/2, -1/2};
ρ =
 1/2 Outer[Times, ψ1, ψ1*] + 1/2 Outer[Times, ψ2, ψ2*] //
  Simplify
{{3/4, 0}, {0, 1/4}}

Tr[ρ.ρ]
5/8
```

---

23. ((Exmple-4))

An attempt to perform a Bell-state measurement on two photons produces a mixed state, one in which the two photons are in the entangled state

$$\frac{1}{\sqrt{2}}[|x,x\rangle + |y,y\rangle]$$

with probability *p* and with probability $(1-p)/2$ in each of the states $|x,x\rangle$ and $|y,y\rangle$. Determine the density matrix for this ensemble using the linear polarization states of the photons as basis states.

((**Solution**))

$$|\psi_1\rangle = \frac{1}{\sqrt{2}}[|x,x\rangle + |y,y\rangle] = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ 0 \\ 1 \end{pmatrix},$$

$$|\psi_2\rangle = |x,x\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \qquad |\psi_3\rangle = |y,y\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

The density operator:

$$\begin{aligned}\hat{\rho} &= p|\psi_1\rangle\langle\psi_1| + \frac{1-p}{2}|\psi_2\rangle\langle\psi_2| + \frac{1-p}{2}|\psi_3\rangle\langle\psi_3| \\ &= \frac{1}{2}\begin{pmatrix} 1 & 0 & 0 & p \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ p & 0 & 0 & 1 \end{pmatrix}\end{aligned}$$

where

$$Tr[\hat{\rho}] = 1$$

$$Tr[\hat{\rho}^2] = \frac{1+p^2}{2}$$

((**Mathematica**))

```
Clear["Global`*"];
expr_* := expr /. Complex[a_, b_] :> Complex[a, -b];
ψ1 = 1/√2 {1, 0, 0, 1}; ψ2 = {1, 0, 0, 0};
ψ3 = {0, 0, 0, 1};

ρ =
 p Outer[Times, ψ1, ψ1] + (1 - p)/2 Outer[Times, ψ2, ψ2] +
   (1 - p)/2 Outer[Times, ψ3, ψ3] // Simplify
```

$$\left\{\left\{\frac{1}{2}, 0, 0, \frac{p}{2}\right\}, \{0, 0, 0, 0\}, \{0, 0, 0, 0\}, \left\{\frac{p}{2}, 0, 0, \frac{1}{2}\right\}\right\}$$

```
ρ // MatrixForm
```

$$\begin{pmatrix} \frac{1}{2} & 0 & 0 & \frac{p}{2} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \frac{p}{2} & 0 & 0 & \frac{1}{2} \end{pmatrix}$$

24. ((Example-5))

Use the density operator formalism to show the probability that a measurement finds two spin-1/2 particles in the state $|+x,+x\rangle$ differs for the pure Bell state,

$$|\Phi^{(+)}\rangle = \frac{1}{\sqrt{2}}[|+z,+z\rangle + |-z,-z\rangle]$$

for which,

$$\hat{\rho}_1 = |\Phi^{(+)}\rangle\langle\Phi^{(+)}|$$

and for the mixed state

$$\hat{\rho}_2 = \frac{1}{2}\left|+z,+z\right\rangle\left\langle+z,+z\right| + \frac{1}{2}\left|-z,-z\right\rangle\left\langle-z,-z\right|$$

Thus, the disagreement between the predictions of quantum mechanics for the entangled state and those consistent with the views of a local realist are apparent without having to resort to Bell inequalities.

((**Solution**))

The Bell state $\left|\Phi^{(+)}\right\rangle$ is given by

$$\left|\Phi^{(+)}\right\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\0\\1\end{pmatrix},$$

and, the first density operator is

$$\hat{\rho}_1 = \left|\Phi^{(+)}\right\rangle\left\langle\Phi^{(+)}\right| = \frac{1}{2}\begin{pmatrix}1&0&0&1\\0&0&0&0\\0&0&0&0\\1&0&0&1\end{pmatrix},$$

for the Bell state.

$$Tr(\hat{\rho}_1^{\ 2}) = 1$$

which means that $\hat{\rho}_1$ is the density operator for the pure state.

When

$$\left|+x,+x\right\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\\1\\1\end{pmatrix},$$

the projection operator is given by

$$\hat{P}_{|+x,+x\rangle} = |+x,+x\rangle\langle +x,+x| = \frac{1}{4}\begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{pmatrix}.$$

Then we have

$$Tr[\hat{P}_{|+x,+x\rangle}\hat{\rho}_1] = \frac{1}{2}.$$

The probability of finding the system in the state $|+x,+x\rangle$ is 1/2.

We now consider the second density operator given by

$$\begin{aligned}\hat{\rho}_2 &= \frac{1}{2}|+z,+z\rangle\langle +z,+z| + \frac{1}{2}|-z,-z\rangle\langle -z,-z| \\ &= \frac{1}{2}\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}\end{aligned}$$

Since

$$Tr(\hat{\rho}_2{}^2) = \frac{1}{2} \text{ (<1).}$$

$\hat{\rho}_2$ is the density operator for the mixed state. We have

$$Tr[\hat{P}_{|+x,+x\rangle}\hat{\rho}_2] = \frac{1}{4}.$$

The probability of finding this system in the state $|+x,+x\rangle$ is 1/4.

((**Mathematica**))

```
Clear["Global`*"]; expr_* := expr /. Complex[a_, b_] :→ Complex[a, -b];
ψxpT = 1/Sqrt[2] {1, 1}; ϕxp = 1/Sqrt[2] (1
                                         1); ϕzp = (1
                                                    0); ϕzn = (0
                                                               1);
ψ11 = 1/Sqrt[2] (KroneckerProduct[ϕzp, ϕzp] + KroneckerProduct[ϕzn, ϕzn]);
ψ1 = Transpose[ψ11][[1]]; ψ21 = KroneckerProduct[ϕxp, ϕxp]; ψ2 = Transpose[ψ21][[1]];
ψ3p1 = KroneckerProduct[ϕzp, ϕzp]; ψ3p = Transpose[ψ3p1][[1]];
ψ3n1 = KroneckerProduct[ϕzn, ϕzn];
ψ3n = Transpose[ψ3n1][[1]];
```

```
ψ11 // MatrixForm
```

$$\begin{pmatrix} \frac{1}{\sqrt{2}} \\ 0 \\ 0 \\ \frac{1}{\sqrt{2}} \end{pmatrix}$$

```
ψ21 // MatrixForm
```

$$\begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}$$

```
ρ1 = Outer[Times, ψ1, ψ1] // Simplify; ρ1 // MatrixForm
```

$$\begin{pmatrix} \frac{1}{2} & 0 & 0 & \frac{1}{2} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \frac{1}{2} & 0 & 0 & \frac{1}{2} \end{pmatrix}$$

```
Tr[ρ1.ρ1]
```

1

```
PX = Outer[Times, ψ2, ψ2] // Simplify;
```

```
PX // MatrixForm
```

$$\begin{pmatrix} \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \end{pmatrix}$$

```
Tr[PX.ρ1]
```

$\frac{1}{2}$

$$\rho 2 = \frac{1}{2}\ \text{Outer[Times, ψ3p, ψ3p]} + \frac{1}{2}\ \text{Outer[Times, ψ3n, ψ3n]};$$

```
ρ2 // MatrixForm
```

$$\begin{pmatrix} \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} \end{pmatrix}$$

```
Tr[ρ2.ρ2]
```

$\frac{1}{2}$

```
Tr[PX.ρ2]
```

$\frac{1}{4}$

25. ((Example-6))

Prove that the state of the form

$$|\psi\rangle_{12} = C_{xy}|x\rangle_1 \otimes |y\rangle_2 + C_{yx}|y\rangle_1 \otimes |x\rangle_2 = \begin{pmatrix} 0 \\ C_{xy} \\ C_{yx} \\ 0 \end{pmatrix}$$

where

$$|C_{xy}|^2 + |C_{yx}|^2 = 1$$

and both coefficients are non-zero, cannot be written as a Kronecker product state

$$|\psi'\rangle_{12} = |\psi\rangle_1 \otimes |\phi\rangle_2$$

with

$$|\psi\rangle_1 = \alpha_x|x\rangle_1 + \alpha_y|y\rangle_1$$

$$|\phi\rangle_2 = \beta_x|x\rangle_2 + \beta_y|y\rangle_2 .$$

((**Solution**))

$$|\psi'\rangle_{12} = |\psi\rangle_1 \otimes |\phi\rangle_2 = \begin{pmatrix} \alpha_x\beta_x \\ \alpha_x\beta_y \\ \alpha_y\beta_x \\ \alpha_y\beta_y \end{pmatrix}$$

Suppose that $|\psi'\rangle_{12} = |\psi\rangle_{12}$. Then we have

$$\alpha_x\beta_x = 0 , \qquad \alpha_y\beta_y = 0 , \qquad C_{xy} = \alpha_x\beta_y , \qquad C_{yx} = \alpha_y\beta_x$$

Then we get

$$C_{xy}C_{yx} = \alpha_x\beta_y\alpha_y\beta_x = \alpha_x\beta_x\alpha_y\beta_y = 0$$

This is not consistent with the assumption that both C_{xy} and C_{yxy} are non-zero.

26. Example ((Townsend))

Consider the state vector

$$|\psi\rangle_{12} = \frac{1}{2}[|x\rangle_1 \otimes |x\rangle_2 + |x\rangle_1 \otimes |y\rangle_2 + |y\rangle_1 \otimes |x\rangle_2 + |y\rangle_1 \otimes |y\rangle_2],$$

describing the polarization of two photons. Show that the reduced density operators

$$\hat{\rho}_1 = Tr_2[\hat{\rho}_{12}], \qquad \hat{\rho}_2 = Tr_1[\hat{\rho}_{12}]$$

describe pure states, where

$$\hat{\rho}_{12} = |\psi\rangle_{1212}\langle\psi|$$

((**Solution**))

The density operator:

$$\hat{\rho}_{12} = \frac{1}{4}\begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{pmatrix}$$

The reduced density operators:

$$\hat{\rho}_1 = Tr_2[\hat{\rho}_{12}] = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}, \qquad \hat{\rho}_2 = Tr_1[\hat{\rho}_{12}] = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$$

Since

$$\hat{\rho}_1^{\,2} = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} = \hat{\rho}_1, \quad \hat{\rho}_2^{\,2} = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} = \hat{\rho}_2$$

the reduced density operators $\hat{\rho}_1$ and $\hat{\rho}_2$ describe pure state.

27.

We consider the density operator (4x4 matrix) in the Hilbert space.

$$\hat{\rho} = \frac{1}{4}(1-\varepsilon)\hat{I}_4 + \varepsilon(|0\rangle \otimes |0\rangle)(\langle 0| \otimes \langle 0|)$$

where ε is a real parameter (0<ε<1). Show that the system is mixed.

((**Solution**))

We examine the property of the density operator.

$$\hat{\rho} = \begin{pmatrix} \varepsilon + \frac{1-\varepsilon}{4} & 0 & 0 & 0 \\ 0 & \frac{1-\varepsilon}{4} & 0 & 0 \\ 0 & 0 & \frac{1-\varepsilon}{4} & 0 \\ 0 & 0 & 0 & \frac{1-\varepsilon}{4} \end{pmatrix}$$

Thus

$$\hat{\rho}^{+} = \hat{\rho}$$

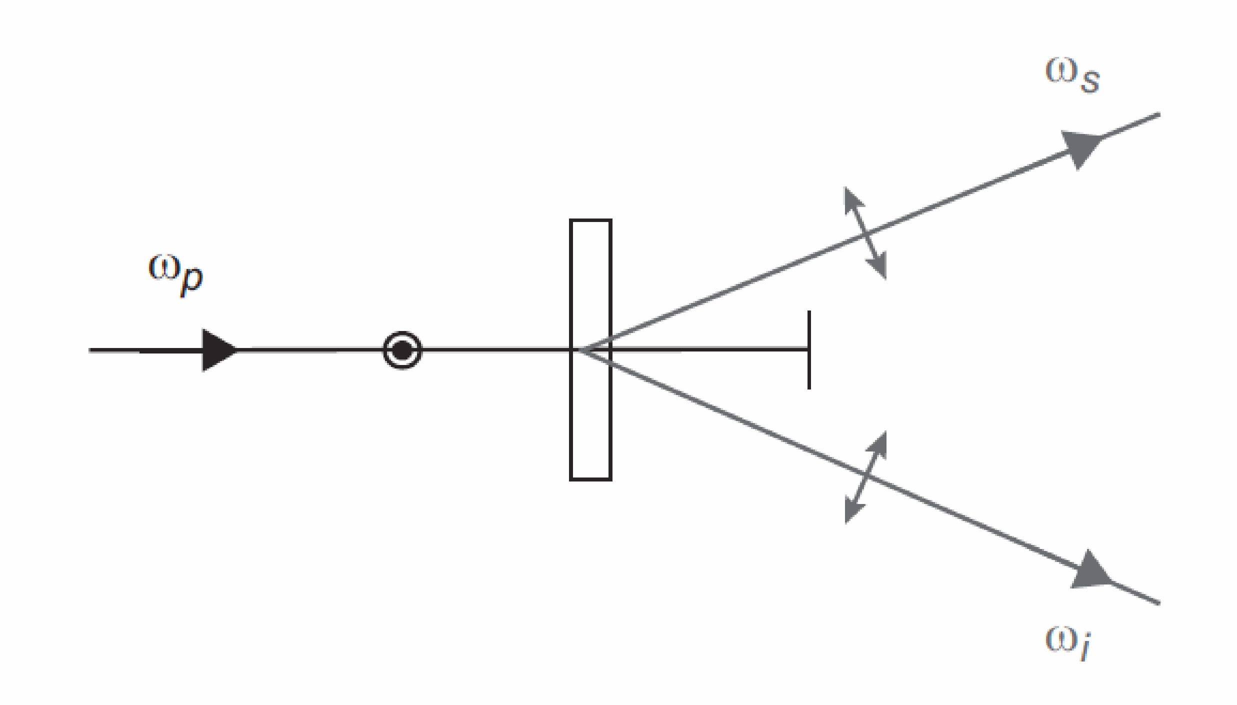
$$Tr[\hat{\rho}^2] = \frac{1+3\varepsilon^2}{4}, \qquad Tr[\hat{\rho}] = 1$$

For $0 < \varepsilon < 1$, we have

$$0 < Tr[\hat{\rho}^2] < 1,$$

which means that the system is mixed.

28. Two Photons system as example



In order to describe the polarization state of the two-photon system shown in Fig., the polarization of each photon must be specified. This polarization state is

$$\left|x,x\right\rangle = \left|x_s\right\rangle \otimes \left|x_i\right\rangle = \begin{pmatrix}1\\0\end{pmatrix} \otimes \begin{pmatrix}1\\0\end{pmatrix} = \begin{pmatrix}1\\0\\0\\0\end{pmatrix}$$

The symbol $\otimes$ denotes the direct product, which combines state vectors in different Hilbert spaces (one for each particle) to create a new vector that specifies the state of the two-particle system in an enlarged Hilbert space.

$$\begin{aligned}\left|+45°, x\right\rangle &= \left|+45°\right\rangle_s \otimes \left|x_i\right\rangle \\ &= \frac{1}{\sqrt{2}}[\left|x_s\right\rangle \otimes \left|x_i\right\rangle + \left|y_s\right\rangle \otimes \left|x_i\right\rangle] \\ &= \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix} \otimes \begin{pmatrix}1\\0\end{pmatrix} \\ &= \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\1\\0\end{pmatrix}\end{aligned}$$

where

$$\left|x_s\right\rangle \otimes \left|x_i\right\rangle = \begin{pmatrix}1\\0\end{pmatrix} \otimes \begin{pmatrix}1\\0\end{pmatrix} = \begin{pmatrix}1\\0\\0\\0\end{pmatrix}$$

$$\left|y_s\right\rangle \otimes \left|y_i\right\rangle = \begin{pmatrix}0\\1\end{pmatrix} \otimes \begin{pmatrix}1\\0\end{pmatrix} = \begin{pmatrix}0\\0\\1\\0\end{pmatrix}$$

$$\begin{aligned}\left|+45°, R\right\rangle &= \left|+45°\right\rangle_s \otimes \left|R\right\rangle_i \\ &= \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix} \otimes \begin{pmatrix}1\\i\end{pmatrix} \\ &= \frac{1}{\sqrt{2}}\begin{pmatrix}1\\i\\1\\i\end{pmatrix}\end{aligned}$$

((**Note**))

$$\left|x\right\rangle = \begin{pmatrix}1\\0\end{pmatrix}, \qquad \left|y\right\rangle = \begin{pmatrix}0\\1\end{pmatrix}$$

$$|+45°\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}, \qquad |+45°\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}$$

$$|R\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\i\end{pmatrix}, \qquad |L\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-i\end{pmatrix}$$

The entangled state

$$|\psi\rangle = \frac{1}{\sqrt{2}}[|x_s\rangle \otimes |x_i\rangle + |y_s\rangle \otimes |y_i\rangle]$$
$$= \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\0\\1\end{pmatrix}$$

$$|x_s\rangle \otimes |y_i\rangle = \begin{pmatrix}1\\0\end{pmatrix} \otimes \begin{pmatrix}0\\1\end{pmatrix} = \begin{pmatrix}0\\1\\0\\0\end{pmatrix}$$

$$|y_s\rangle \otimes |x_i\rangle = \begin{pmatrix}0\\1\end{pmatrix} \otimes \begin{pmatrix}1\\0\end{pmatrix} = \begin{pmatrix}0\\0\\1\\0\end{pmatrix}$$

$$|y_s\rangle \otimes |y_i\rangle = \begin{pmatrix}0\\1\end{pmatrix} \otimes \begin{pmatrix}0\\1\end{pmatrix} = \begin{pmatrix}0\\0\\0\\1\end{pmatrix}$$

$$|x', x\rangle = |+45°, x\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix} \otimes \begin{pmatrix}1\\0\end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\1\\0\end{pmatrix}$$

$$\left|x',y\right\rangle = \left|+45°,y\right\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}\otimes\begin{pmatrix}0\\1\end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix}0\\1\\0\\1\end{pmatrix}$$

$$\left|y,+45°\right\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}0\\1\end{pmatrix}\otimes\begin{pmatrix}1\\1\end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix}0\\0\\1\\1\end{pmatrix}$$

$$\left|+45°,R\right\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}\otimes\begin{pmatrix}1\\i\end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\i\\1\\i\end{pmatrix}$$

$$\left|+45°,L\right\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}\otimes\begin{pmatrix}1\\-i\end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-i\\1\\-i\end{pmatrix}$$

$$\left|+45°,+45°\right\rangle = \frac{1}{2}\begin{pmatrix}1\\1\end{pmatrix}\otimes\begin{pmatrix}1\\1\end{pmatrix} = \frac{1}{2}\begin{pmatrix}1\\1\\1\\1\end{pmatrix}$$

29. HV polarization operator:

$$[\hat{P}^s_{HV},\hat{P}^i_{HV}] = 0$$

$$\hat{P}_{HV} = |x\rangle\langle x| - |y\rangle\langle y| = \begin{pmatrix}1 & 0\\0 & -1\end{pmatrix},$$

where

$$|x\rangle\langle x| = \begin{pmatrix}1\\0\end{pmatrix}\begin{pmatrix}1 & 0\end{pmatrix} = \begin{pmatrix}1 & 0\\0 & 0\end{pmatrix},$$

$$|y\rangle\langle y| = \begin{pmatrix} 0 \\ 1 \end{pmatrix}(0 \quad 1) = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

((Example-1))

Calculate the action of operator $\hat{P}_{HV}^{s}$, $\hat{P}_{HV}^{i}$, and $\hat{P}_{HV}^{si}$ on the state $|V,+45°\rangle$

$$|y,+45°\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 0 \\ 1 \\ 1 \end{pmatrix}$$

$$|y,-45°\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ -1 \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 0 \\ 1 \\ -1 \end{pmatrix}$$

$$\hat{P}_{HV}^{s} = \hat{P}_{HV} \otimes \hat{1} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix},$$

$$\hat{P}_{HV}^{2} = \hat{1} \otimes \hat{P}_{HV} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix},$$

$$\hat{P}_{HV}^{s} \otimes \hat{P}_{HV}^{i} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

$$(\hat{P}_{HV}^{s} \otimes \hat{1}_{i})|y,+45°\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 0 \\ -1 \\ -1 \end{pmatrix} = -|y,+45°\rangle$$

$$(\hat{1}_s \otimes \hat{P}_{HV})|y,+45°\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 0 \\ 1 \\ -1 \end{pmatrix} = |y,-45°\rangle$$

$$\hat{P}_{HV}^{si}|y,+45°\rangle = (\hat{P}_{HV}^{s} \otimes \hat{P}_{HV}^{i})|y,+45°\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 0 \\ -1 \\ 1 \end{pmatrix} = -|y,-45°\rangle$$

30. Problems and solutions

Compare the density operators that correspond to the following two states: (a) a superposition that consists of equal parts $|x,x\rangle$ and $|y,y\rangle$ (assuming a relative phase of zero), and (b) a mixture that consists of equal parts $|x,x\rangle$ and $|y,y\rangle$.

((**Solution**))

(a) The state vector corresponding to this pure state is

$$\begin{aligned}
|\psi\rangle &= \frac{1}{\sqrt{2}}(|x,x\rangle + |y,y\rangle \\
&= \frac{1}{\sqrt{2}}(|x\rangle \otimes |x\rangle + |y\rangle \otimes |y\rangle \\
&= \frac{1}{\sqrt{2}}[\begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix}] \\
&= \frac{1}{\sqrt{2}}[\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}] \\
&= \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ 0 \\ 1 \end{pmatrix}
\end{aligned}$$

Its corresponding density operator is

$$\hat{\rho} = |\psi\rangle\langle\psi| = \frac{1}{2}\begin{pmatrix}1\\0\\0\\1\end{pmatrix}\begin{pmatrix}1 & 0 & 0 & 1\end{pmatrix} = \frac{1}{2}\begin{pmatrix}1 & 0 & 0 & 1\\0 & 0 & 0 & 0\\0 & 0 & 0 & 0\\1 & 0 & 0 & 1\end{pmatrix}$$

(b) The density operator corresponding to this mixed state is

$$\hat{\rho} = \frac{1}{2}|x,x\rangle\langle x,x| + \frac{1}{2}|y,y\rangle\langle y,y|$$

$$= \frac{1}{2}[\begin{pmatrix}1\\0\\0\\0\end{pmatrix}\begin{pmatrix}1 & 0 & 0 & 0\end{pmatrix} + \begin{pmatrix}0\\0\\0\\1\end{pmatrix}\begin{pmatrix}0 & 0 & 0 & 1\end{pmatrix}]$$

$$= \frac{1}{2}[\begin{pmatrix}1 & 0 & 0 & 0\\0 & 0 & 0 & 0\\0 & 0 & 0 & 0\\0 & 0 & 0 & 0\end{pmatrix} + \begin{pmatrix}0 & 0 & 0 & 0\\0 & 0 & 0 & 0\\0 & 0 & 0 & 0\\0 & 0 & 0 & 1\end{pmatrix}]$$

$$= \frac{1}{2}\begin{pmatrix}1 & 0 & 0 & 0\\0 & 0 & 0 & 0\\0 & 0 & 0 & 0\\0 & 0 & 0 & 1\end{pmatrix}$$

Clearly these are different; the density operator corresponding to the pure state has two more terms. These extra terms, which intermingle the states $|x,x\rangle$ and $|y,y\rangle$ contributions, contain information about the entanglement between the states.

31. Problems and solutions

For a two-photon system prepared in an equal mixture of states $|x,x\rangle$ and $|y,y\rangle$ determine the probability that the signal photon is measured to be polarized along +45°, given that the idler photon is found to be polarized along this same direction. The density operator corresponding to this state is given by

$$\hat{\rho} = \frac{1}{2}|x,x\rangle\langle x,x| + \frac{1}{2}|y,y\rangle\langle y,y| = \frac{1}{2}\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

We want to find $P(+45°_s \mid +45°_i)$, which is

$$P(+45°_s \mid +45°_i) = \frac{P(+45°_s, +45°_i)}{P(+45°_i)}$$

((**Solution**))

$$\begin{aligned} P(+45°_s, +45°_i) &= Tr[|+45°_s, +45°_i\rangle\langle +45°_s, +45°_i|\hat{\rho}] \\ &= Tr[\frac{1}{2}\left(\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}\right)\frac{1}{4}\begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{pmatrix}] \\ &= \frac{1}{8}Tr\begin{pmatrix} 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 \end{pmatrix} \\ &= \frac{1}{4} \end{aligned}$$

where

$$|+45°, +45°\rangle = \frac{1}{2}\begin{pmatrix} 1 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 1 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}$$

$$|+45°_s, +45°_i\rangle\langle +45°_s, +45°_i| = \frac{1}{4}\begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}\begin{pmatrix} 1 & 1 & 1 & 1 \end{pmatrix} = \frac{1}{4}\begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{pmatrix}$$

We also have

$$P(+45°_i) = Tr[(\hat{1}_s \otimes |+45°_i\rangle\langle +45°_i|)\hat{\rho}]$$
$$= \frac{1}{4} Tr[\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 \end{pmatrix}]$$
$$= \frac{1}{4} Tr[\begin{pmatrix} 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 \end{pmatrix}]$$
$$= \frac{1}{2}$$

where

$$\hat{1}_s \otimes |+45°_i\rangle\langle +45°_i|) = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 \end{pmatrix}$$

$$|+45°_i\rangle\langle +45°_i| = \frac{1}{2}\begin{pmatrix} 1 \\ 1 \end{pmatrix}\begin{pmatrix} 1 & 1 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$$

Using the values of $P(+45°_i)$ and $P(+45°_s, +45°_i)$, we get

$$P(+45°_s \,|\, +45°_i) = \frac{P(+45°_s, +45°_i)}{P(+45°_i)} = \frac{\frac{1}{4}}{\frac{1}{2}} = \frac{1}{2}.$$

((**Note**)) **Bayes' theorem**

Bayes' formula is state mathematically as follows.

$P(a \,|\, b)$ (conditional probability) is given by

$$P(a \mid b) = \frac{P(a,b)}{P(b)} = \frac{P(a)P(b \mid a)}{P(b)}$$

where a and b are events. $P(a)$ and $P(b)$ are the probabilities of a and b without regard to each other. $P(a \mid b)$, which is a conditional probability, is the probability of observing event a given that b is true. $P(b \mid a)$, which is a conditional probability, is the probability of observing event b given that a is true.

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APPENDIX - I Definition of the KroneckerProduct $\otimes$

(a)

$$\hat{A} = \begin{pmatrix} a_1 \\ a_2 \end{pmatrix}, \qquad \hat{B} = \begin{pmatrix} b_1 \\ b_2 \end{pmatrix}$$

$$\hat{A}\otimes\hat{B}=\begin{pmatrix}a_1\\a_2\end{pmatrix}\otimes\begin{pmatrix}b_1\\b_2\end{pmatrix}=\begin{pmatrix}a_1B\\a_2B\end{pmatrix}=\begin{pmatrix}a_1b_1\\a_1b_2\\a_2b_1\\a_2b_2\end{pmatrix}$$

(b)

$$\hat{A}=\begin{pmatrix}a_{11}&a_{12}\\a_{21}&a_{22}\end{pmatrix},\qquad \hat{B}=\begin{pmatrix}b_{11}&b_{12}\\b_{21}&b_{22}\end{pmatrix}$$

$$\hat{A}\otimes\hat{B}=\begin{pmatrix}a_{11}\hat{B}&a_{12}\hat{B}\\a_{21}\hat{B}&a_{22}\hat{B}\end{pmatrix}=\begin{pmatrix}a_{11}b_{11}&a_{11}b_{12}&a_{12}b_{11}&a_{12}b_{12}\\a_{11}b_{21}&a_{11}b_{22}&a_{12}b_{21}&a_{12}b_{22}\\a_{21}b_{11}&a_{21}b_{12}&a_{22}b_{11}&a_{22}b_{12}\\a_{21}b_{21}&a_{21}b_{22}&a_{22}b_{21}&a_{22}b_{22}\end{pmatrix}$$

APPENDIX - II Formula related to the Kronecker product

$$Tr(\hat{A}\hat{B})=Tr(\hat{B}\hat{A}) \tag{1}$$

$$Tr(\hat{A}\hat{B}\hat{C})=Tr(\hat{B}\hat{C}\hat{A})=Tr(\hat{C}\hat{A}\hat{B}) \tag{2}$$

$$Tr[|a\rangle\langle b|]=\langle b|a\rangle \tag{3}$$

$$Tr[a\hat{A}+b\hat{B}]=aTr[\hat{A}]+bTr[\hat{B}] \tag{4}$$

$$|a_1,b_2\rangle\langle c_1,d_2|=(|a_1\rangle\otimes|b_2\rangle)(\langle c_1|\otimes\langle d_2|)=(|a_i\rangle\langle c_1|)_1\otimes(|b_2\rangle\langle d_2|) \tag{5}$$

$$Tr[\hat{A}\otimes\hat{B}]=Tr[\hat{B}\otimes\hat{A}]=Tr[\hat{A}]Tr[\hat{B}] \tag{6}$$

$$Tr_2(\hat{A}_1\otimes\hat{B}_2)=\hat{A}_1Tr_2(\hat{B}_2) \tag{7}$$

$$Tr_1(\hat{A}_1\otimes\hat{B}_2)=\hat{B}_2Tr_1(\hat{A}_1) \tag{8}$$

$$\langle A_1\rangle=Tr_1[\hat{A}_1\hat{\rho}_1]=Tr_{12}[(\hat{A}_1\otimes\hat{1}_2)\hat{\rho}_{12}] \tag{9}$$

$$\langle A_2 \rangle = Tr_2[\hat{A}_2\hat{\rho}_2] = Tr_{12}[(\hat{1}_1 \otimes \hat{A}_2)\hat{\rho}_{12}] \quad (10)$$

$$(|a_1, b_2\rangle\langle c_1, d_2|)(|e_1, f_2\rangle\langle g_1, h_2|) = (|a_1, b_2\rangle\langle g_1, h_2|)\langle c_1|e_1\rangle\langle d_2|f_2\rangle \quad (11)$$

Comment on the formula (5)

$$|a_1, b_2\rangle\langle c_1, d_2| = (|a_1\rangle \otimes |b_2\rangle)(\langle c_1| \otimes \langle d_2|) = (|a_i\rangle\langle c_1|)_1 \otimes (|b_2\rangle\langle d_2|)$$

Here we show that

$$\begin{aligned} |+x,+z\rangle\langle +x,+z| &= (|+x\rangle \otimes |+z\rangle)(\langle +x| \otimes \langle +z|) \\ &= (|+x\rangle\langle +x|) \otimes (|+z\rangle\langle +z|) \end{aligned}$$

as a part of proof of the above formula.

$$|+x\rangle \otimes |+z\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix} \otimes \begin{pmatrix}1\\0\end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\1\\0\end{pmatrix}$$

$$\langle +x| \otimes \langle +z| = \frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\end{pmatrix} \otimes \begin{pmatrix}1 & 0\end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix}1 & 0 & 1 & 0\end{pmatrix}$$

$$(|+x\rangle \otimes |+z\rangle)(\langle +x| \otimes \langle +z| = \frac{1}{2}\begin{pmatrix}1\\0\\1\\0\end{pmatrix}\begin{pmatrix}1 & 0 & 1 & 0\end{pmatrix} = \frac{1}{2}\begin{pmatrix}1 & 0 & 1 & 0\\0 & 0 & 0 & 0\\1 & 0 & 1 & 0\\0 & 0 & 0 & 0\end{pmatrix}$$

Note that

$$|+x\rangle\langle +x| = \frac{1}{2}\begin{pmatrix}1\\1\end{pmatrix}\begin{pmatrix}1 & 1\end{pmatrix} = \frac{1}{2}\begin{pmatrix}1 & 1\\1 & 1\end{pmatrix}$$

$$|+z\rangle\langle+z| = \begin{pmatrix} 1 \\ 0 \end{pmatrix}\begin{pmatrix} 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

Then we have

$$(|+x\rangle\langle+x|)\otimes(|+z\rangle\langle+z|) = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}\otimes\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

Comment on formula (6)

$$Tr[\hat{A}\otimes\hat{B}] = Tr[\hat{B}\otimes\hat{A}] = Tr[\hat{A}]Tr[\hat{B}]$$

((**Mathematica**))

```
Clear["Global`*"]; A1 = ( a11 a12 a13
                          a21 a22 a23
                          a31 a32 a33 );

B1 = ( b11 b12 b13
       b21 b22 b23
       b31 b32 b33 );

h1 = Tr[KroneckerProduct[A1, B1]] // Factor

(a11 + a22 + a33) (b11 + b22 + b33)

h2 = Tr[A1] Tr[B1]

(a11 + a22 + a33) (b11 + b22 + b33)

h1 - h2

0
```

Comment on Formula (9) and (10)

$$Tr_1[\hat{A}_1\hat{\rho}_1] = Tr_{12}[(\hat{A}_1\otimes\hat{1}_2)\hat{\rho}_{12}]$$

We show that

$$\langle S_{x1}\rangle = Tr_1[\hat{S}_{x1}\hat{\rho}_1] = Tr_{1,2}[(\hat{S}_{x1}\otimes\hat{1}_2)\hat{\rho}_{12}]$$

where

$$\hat{S}_{x1}\to\hat{S}_{x1}\otimes\hat{1}_2, \qquad \hat{\rho}_1\to\hat{\rho}_{12}$$

((**Proof**))
For example, we have the density operator

$$\begin{aligned}\hat{\rho}_{12} &= |+x,+z\rangle\langle +x,+z| \\ &= \frac{1}{2}\begin{pmatrix}1\\0\\1\\0\end{pmatrix}\begin{pmatrix}1 & 0 & 1 & 0\end{pmatrix} \\ &= \frac{1}{2}\begin{pmatrix}1 & 0 & 1 & 0\\0 & 0 & 0 & 0\\1 & 0 & 1 & 0\\0 & 0 & 0 & 0\end{pmatrix}\end{aligned}$$

The reduced density operator is

$$\begin{aligned}\hat{\rho}_1 &= Tr_2[|+x,+z\rangle\langle +x,+z|] \\ &= Tr_2[(|+x\rangle\langle +x|)\otimes(|+z\rangle\langle +z|] \\ &= (|+x\rangle\langle +x|)Tr_2[|+z\rangle\langle +z]| \\ &= |+x\rangle\langle +x| \\ &= \frac{1}{2}\begin{pmatrix}1 & 1\\1 & 1\end{pmatrix}\end{aligned}$$

$$\begin{aligned}\hat{\rho}_2 &= Tr_1[|+x,+z\rangle\langle +x,+z|] \\ &= (|+z\rangle\langle +z|)Tr_2[|+x\rangle\langle +x]| \\ &= |+z\rangle\langle +z| \\ &= \begin{pmatrix}1 & 0\\0 & 0\end{pmatrix}\end{aligned}$$

where

$$\left|+x,+z\right\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}\otimes\begin{pmatrix}1\\0\end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\1\\0\end{pmatrix}$$

We now calculate the average value.

$$\left\langle S_{x1}\right\rangle = Tr_1[\hat{\rho}_1\hat{S}_{x1}] = \frac{\hbar}{2}$$

where

$$\hat{\rho}_1\hat{S}_{x1} = \frac{1}{2}\begin{pmatrix}1 & 1\\1 & 1\end{pmatrix}\frac{\hbar}{2}\begin{pmatrix}0 & 1\\1 & 0\end{pmatrix} = \frac{\hbar}{4}\begin{pmatrix}1 & 1\\1 & 1\end{pmatrix}$$

We also calculate

$$\begin{aligned}\left\langle S_{x1}\right\rangle &= Tr[\hat{\rho}_{12}(\hat{S}_{x1}\otimes\hat{1}_2)]\\ &= \frac{\hbar}{4}Tr[\begin{pmatrix}1 & 0 & 1 & 0\\0 & 0 & 0 & 0\\1 & 0 & 1 & 0\\0 & 0 & 0 & 0\end{pmatrix}\begin{pmatrix}0 & 0 & 1 & 0\\0 & 0 & 0 & 1\\1 & 0 & 0 & 0\\0 & 1 & 0 & 0\end{pmatrix}]\\ &= \frac{\hbar}{4}Tr\begin{pmatrix}1 & 0 & 1 & 0\\0 & 0 & 0 & 0\\1 & 0 & 1 & 0\\0 & 0 & 0 & 0\end{pmatrix}\\ &= \frac{\hbar}{2}\end{aligned}$$

or

$$\begin{aligned}\langle S_{x1}\rangle &= Tr[|+x\rangle\langle +x|\hat{S}_x] \\ &= Tr[\hat{S}_x|+x\rangle\langle +x|] \\ &= \frac{\hbar}{2}Tr[|+x\rangle\langle +x|] \\ &= \frac{\hbar}{2}\langle +x|+x\rangle \\ &= \frac{\hbar}{2}\end{aligned}$$

where

$$\hat{S}_{x1}\otimes\hat{1}_2 = \frac{\hbar}{2}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\otimes\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix}0 & 0 & 1 & 0\\ 0 & 0 & 0 & 1\\ 1 & 0 & 0 & 0\\ 0 & 1 & 0 & 0\end{pmatrix}$$

APPENDIX

A. Partial trace and Kronecker product

$$Tr[|a\rangle\langle b|] = \langle b|a\rangle .$$

$$\begin{aligned}Tr[(|a_1\rangle\langle a_2|)\otimes|b_1\rangle\langle b_2|)] &= Tr[\hat{A}\otimes\hat{B}] \\ &= Tr[\hat{A}]Tr[\hat{B}] \\ &= Tr[|a_1\rangle\langle a_2|]Tr[|b_1\rangle\langle b_2|] \\ &= \langle a_2|a_1\rangle\langle b_2|b_1\rangle\end{aligned}$$

$$Tr[\hat{A}\otimes\hat{B}] = Tr[\hat{A}]Tr[\hat{B}] .$$

$$Tr_B[\hat{A}\otimes\hat{B}] = \hat{A}Tr_B[\hat{B}] .$$

$$Tr_A[\hat{A}\otimes\hat{B}] = \hat{B}Tr_A[\hat{A}] .$$

((**Note**)) Brief proof

$$
\begin{aligned}
Tr[|a\rangle\langle b|] &= \sum_n \langle n|a\rangle\langle b|n\rangle \\
&= \sum_n \langle b|n\rangle\langle n|a\rangle \qquad \text{(closure relation)} \\
&= \langle b|a\rangle
\end{aligned}
$$

$$
\begin{aligned}
Tr[|a\rangle\langle b|\hat{A}] &= \sum_n \langle n|a\rangle\langle b|\hat{A}|n\rangle \\
&= \sum_n \langle b|\hat{A}|n\rangle\langle n|a\rangle \\
&= \langle b|\hat{A}|a\rangle
\end{aligned}
$$

$$
\begin{aligned}
\hat{A}\otimes\hat{B} &= \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \otimes \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} \\
&= \begin{pmatrix} a_{11}B & a_{12}B \\ a_{21}B & a_{22}B \end{pmatrix} \\
&= \begin{pmatrix} a_{11}b_{11} & a_{11}b_{12} & a_{12}b_{11} & a_{12}b_{12} \\ a_{11}b_{21} & a_{11}b_{22} & a_{12}b_{21} & a_{12}b_{22} \\ a_{21}b_{11} & a_{21}b_{12} & a_{22}b_{11} & a_{22}b_{12} \\ a_{21}b_{21} & a_{21}b_{22} & a_{22}b_{21} & a_{22}b_{22} \end{pmatrix}
\end{aligned}
$$

$$
\begin{aligned}
Tr[\hat{A}\otimes\hat{B}] &= Tr[\begin{pmatrix} a_{11}B & a_{12}B \\ a_{21}B & a_{22}B \end{pmatrix}] \\
&= Tr_{AB}[\begin{pmatrix} a_{11}B & a_{12}B \\ a_{21}B & a_{22}B \end{pmatrix}] \\
&= Tr_A \begin{pmatrix} a_{11}Tr_B[\hat{B}] & a_{12}Tr_B[\hat{B}] \\ a_{21}Tr_B[\hat{B}] & a_{22}Tr_B[\hat{B}] \end{pmatrix} \\
&= Tr_A \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} Tr_B[\hat{B}] \\
&= Tr_A[\hat{A}]Tr_B[\hat{B}]
\end{aligned}
$$

$$Tr_B[\hat{A}\otimes\hat{B}] = Tr_B[\begin{pmatrix} a_{11}B & a_{12}B \\ a_{21}B & a_{22}B \end{pmatrix}]$$
$$= \begin{pmatrix} a_{11}Tr_B[\hat{B}] & a_{12}Tr_B[\hat{B}] \\ a_{21}Tr_B[\hat{B}] & a_{22}Tr_B[\hat{B}] \end{pmatrix}$$
$$= \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} Tr_B[\hat{B}]$$
$$= \hat{A}Tr_B[\hat{B}]$$

((**Note**)) Formula of Kronecker product

$$(\hat{A}_1\otimes\hat{A}_2)(|\psi_1\rangle\otimes|\psi_2\rangle) = \hat{A}_1|\psi_1\rangle\otimes\hat{A}_2|\psi_2\rangle .$$

$$(\hat{A}_1\otimes\hat{A}_2)(\hat{B}_1\otimes\hat{B}_2) = (\hat{A}_1\otimes\hat{B}_1)(\hat{A}_2\otimes\hat{B}_2) .$$

$$(\hat{A}\otimes\hat{B})^{-1} = \hat{A}^{-1}\otimes\hat{B}^{-1} .$$

$$(\hat{A}\otimes\hat{B})^{+} = \hat{A}^{+}\otimes\hat{B}^{+}$$

$$(\hat{A}\otimes\hat{B})^{*} = \hat{A}^{*}\otimes\hat{B}^{*}$$

$$(\hat{A}\otimes\hat{B})^{T} = \hat{A}^{T}\otimes\hat{B}^{T}$$

$$\det(\hat{A}\otimes\hat{B}) = \det(\hat{A})\det(\hat{B})$$

$$\exp(\hat{A}\otimes\hat{B}) = \exp(\hat{A})\otimes\exp(\hat{B})$$

$$\hat{A}\otimes\hat{B} \neq \hat{B}\otimes\hat{A}$$

These relations may be reasonable since the site of the particle related to operator $\hat{A}$ is different from those related to $\hat{B}$.

REFERENCES:

A. Graham, Kronecker Products and Matrix Calculus with Applications (Ellis Horwood, 1981)

APPENDIX Mathematica Program of partial trace

I make a Mathematica program for the partial trace for 8x8 matrix and 4x4 matrix, by using the matrix manipulation (switching between rows, and switching between columns). The programs are named as PartialTr81, PartialTr82, and PartialTr83 for the 8x8 matrix, and PartialTr41 and PartialTr42, for the 4x4 matrix.

Program for the partial trace for 8x8 and 4x4 matrix

PartialTr81, PartialTr82, PartialTr83

ρ12=Tr3[ρ123], ρ23=Tr1[ρ123], ρ13=Tr2[ρ123],

PartialTr41, PartialTr42

Tr1[ρ12], Tr2[ρ12]

```
Clear["Gobal`"];
PartialTr41[ρ1_] := Module[{A1,  K1,  K2,  K12}, A1 = ρ1;
  K1 = A1[[{1, 2}, {1, 2}]]; K2 = A1[[{3, 4}, {3, 4}]];
  K12 = K1 + K2];
PartialTr42[ρ1_] :=
 Module[{A1,  K1,  K2,  K12}, A1 = ρ1;
  A1[[All, {2, 3}]] = A1[[All, {3, 2}]];
  A1[[{2, 3}]] = A1[[{3, 2}]];
  K1 = A1[[{1, 2}, {1, 2}]]; K2 = A1[[{3, 4}, {3, 4}]];
  K12 = K1 + K2];
```

```
PartialTr81[ρ1_] := Module[{A1,  K1,  K2,  K12}, A1 = ρ1;
  A1 = ρ1; K1 = A1[[{1, 2,  3, 4}, {1, 2, 3, 4}]];
  K2 = A1[[{5, 6, 7, 8}, {5, 6, 7, 8}]]; K12 = K1 + K2];
PartialTr82[ρ1_] :=
 Module[{A1,  A2,  K1,  K2,  K12}, A1 = ρ1;
  A2 = ρ1; A1[[All, {3, 5}]] = A1[[All, {5, 3}]];
  A1[[All, {4, 6}]] = A1[[All, {6, 4}]];
  A1[[{3, 5}]] = A1[[{5, 3}]];
  A1[[{4, 6}]] = A1[[{6, 4}]];
  A2[[All, {3, 5}]] = A2[[All, {5, 3}]];
  A2[[All,  {4, 6}]] = A2[[All,  {6, 4}]];
  A2[[{3, 5}]] = A2[[{5, 3}]];
  A2[[{4, 6}]] = A2[[{6, 4}]];
  K1 = A1[[{1, 2,  3, 4}, {1, 2, 3, 4}]];
  K2 = A2[[{5, 6, 7, 8}, {5, 6, 7, 8}]]; K12 = K1 + K2];
```

```
PartialTr83[ρ1_] :=
 Module[{A1, A2, K1, K2, K12}, A1 = ρ1;
  A2 = ρ1; A1[[All, {2, 3}]] = A1[[All, {3, 2}]];
  A1[[All, {3, 5}]] = A1[[All, {5, 3}]];
  A1[[All, {4, 7}]] = A1[[All, {7, 4}]];
  A1[[{2, 3}]] = A1[[{3, 2}]];
  A1[[{5, 3}]] = A1[[{3, 5}]];
  A1[[{6, 4}]] = A1[[{4, 6}]];
  A2[[All, {6, 7}]] = A2[[All, {7, 6}]];
  A2[[All, {2, 5}]] = A2[[All, {5, 2}]];
  A2[[All, {4, 6}]] = A2[[All, {6, 4}]];
  A2[[{6, 7}]] = A2[[{7, 6}]];
  A2[[{4, 6}]] = A2[[ {6, 4}]];
  A2[[{2, 5}]] = A2[[{5, 2}]];
  K1 = A1[[{1, 2,  3, 4}, {1, 2, 3, 4}]];
  K2 = A2[[{5, 6, 7, 8}, {5, 6, 7, 8}]]; K12 = K1 + K2];
```

((Example)) GHZ state

```
ψ = 1/√2 (1, 0, 0, 0, 0, 0, 0, 1)ᵀ; ψH = Transpose[ψ]
```

$$\left\{\left\{\frac{1}{\sqrt{2}}, 0, 0, 0, 0, 0, 0, \frac{1}{\sqrt{2}}\right\}\right\}$$

```
ρ = ψ.ψH; ρ // MatrixForm
```

$$\begin{pmatrix} \frac{1}{2} & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{2} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{2} & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{2} \end{pmatrix}$$

```
ρ12 = PartialTr83[ρ]
```

$\left\{\left\{\frac{1}{2}, 0, 0, 0\right\}, \{0, 0, 0, 0\}, \{0, 0, 0, 0\}, \left\{0, 0, 0, \frac{1}{2}\right\}\right\}$

```
ρ13 = PartialTr82[ρ]
```

$\left\{\left\{\frac{1}{2}, 0, 0, 0\right\}, \{0, 0, 0, 0\}, \{0, 0, 0, 0\}, \left\{0, 0, 0, \frac{1}{2}\right\}\right\}$

```
ρ23 = PartialTr81[ρ]
```

$\left\{\left\{\frac{1}{2}, 0, 0, 0\right\}, \{0, 0, 0, 0\}, \{0, 0, 0, 0\}, \left\{0, 0, 0, \frac{1}{2}\right\}\right\}$

```
ρ1 = PartialTr42[ρ12]
```

$\left\{\left\{\frac{1}{2}, 0\right\}, \left\{0, \frac{1}{2}\right\}\right\}$

```
ρ2 = PartialTr42[ρ12]
```

$\left\{\left\{\frac{1}{2}, 0\right\}, \left\{0, \frac{1}{2}\right\}\right\}$

((**Example-2**)) Another GHZ state

GHZ sate Density operator, Partial trace

```
ψ = 1/2 (α, β, β, α, α, -β, -β, α)ᵀ; ψH = Transpose[ψ] /. {α → α1, β → β1}
```

$$\left\{\left\{\frac{\alpha 1}{2}, \frac{\beta 1}{2}, \frac{\beta 1}{2}, \frac{\alpha 1}{2}, \frac{\alpha 1}{2}, -\frac{\beta 1}{2}, -\frac{\beta 1}{2}, \frac{\alpha 1}{2}\right\}\right\}$$

```
ψH.ψ
```

$$\{\{\alpha\,\alpha 1 + \beta\,\beta 1\}\}$$

```
ρ = ψ.ψH; ρ // MatrixForm
```

$$\begin{pmatrix}
\frac{\alpha\,\alpha 1}{4} & \frac{\alpha\,\beta 1}{4} & \frac{\alpha\,\beta 1}{4} & \frac{\alpha\,\alpha 1}{4} & \frac{\alpha\,\alpha 1}{4} & -\frac{\alpha\,\beta 1}{4} & -\frac{\alpha\,\beta 1}{4} & \frac{\alpha\,\alpha 1}{4} \\
\frac{\alpha 1\,\beta}{4} & \frac{\beta\,\beta 1}{4} & \frac{\beta\,\beta 1}{4} & \frac{\alpha 1\,\beta}{4} & \frac{\alpha 1\,\beta}{4} & -\frac{\beta\,\beta 1}{4} & -\frac{\beta\,\beta 1}{4} & \frac{\alpha 1\,\beta}{4} \\
\frac{\alpha 1\,\beta}{4} & \frac{\beta\,\beta 1}{4} & \frac{\beta\,\beta 1}{4} & \frac{\alpha 1\,\beta}{4} & \frac{\alpha 1\,\beta}{4} & -\frac{\beta\,\beta 1}{4} & -\frac{\beta\,\beta 1}{4} & \frac{\alpha 1\,\beta}{4} \\
\frac{\alpha\,\alpha 1}{4} & \frac{\alpha\,\beta 1}{4} & \frac{\alpha\,\beta 1}{4} & \frac{\alpha\,\alpha 1}{4} & \frac{\alpha\,\alpha 1}{4} & -\frac{\alpha\,\beta 1}{4} & -\frac{\alpha\,\beta 1}{4} & \frac{\alpha\,\alpha 1}{4} \\
\frac{\alpha\,\alpha 1}{4} & \frac{\alpha\,\beta 1}{4} & \frac{\alpha\,\beta 1}{4} & \frac{\alpha\,\alpha 1}{4} & \frac{\alpha\,\alpha 1}{4} & -\frac{\alpha\,\beta 1}{4} & -\frac{\alpha\,\beta 1}{4} & \frac{\alpha\,\alpha 1}{4} \\
-\frac{\alpha 1\,\beta}{4} & -\frac{\beta\,\beta 1}{4} & -\frac{\beta\,\beta 1}{4} & -\frac{\alpha 1\,\beta}{4} & -\frac{\alpha 1\,\beta}{4} & \frac{\beta\,\beta 1}{4} & \frac{\beta\,\beta 1}{4} & -\frac{\alpha 1\,\beta}{4} \\
-\frac{\alpha 1\,\beta}{4} & -\frac{\beta\,\beta 1}{4} & -\frac{\beta\,\beta 1}{4} & -\frac{\alpha 1\,\beta}{4} & -\frac{\alpha 1\,\beta}{4} & \frac{\beta\,\beta 1}{4} & \frac{\beta\,\beta 1}{4} & -\frac{\alpha 1\,\beta}{4} \\
\frac{\alpha\,\alpha 1}{4} & \frac{\alpha\,\beta 1}{4} & \frac{\alpha\,\beta 1}{4} & \frac{\alpha\,\alpha 1}{4} & \frac{\alpha\,\alpha 1}{4} & -\frac{\alpha\,\beta 1}{4} & -\frac{\alpha\,\beta 1}{4} & \frac{\alpha\,\alpha 1}{4}
\end{pmatrix}$$

```
ρ23 = PartialTr81[ρ]
```

$$\left\{\left\{\frac{\alpha\,\alpha 1}{2}, 0, 0, \frac{\alpha\,\alpha 1}{2}\right\}, \left\{0, \frac{\beta\,\beta 1}{2}, \frac{\beta\,\beta 1}{2}, 0\right\}, \left\{0, \frac{\beta\,\beta 1}{2}, \frac{\beta\,\beta 1}{2}, 0\right\}, \left\{\frac{\alpha\,\alpha 1}{2}, 0, 0, \frac{\alpha\,\alpha 1}{2}\right\}\right\}$$

```
ρ3 = PartialTr41[ρ23] // Simplify
```

$$\left\{\left\{\frac{1}{2}(\alpha\,\alpha 1 + \beta\,\beta 1), 0\right\}, \left\{0, \frac{1}{2}(\alpha\,\alpha 1 + \beta\,\beta 1)\right\}\right\}$$

```
ρ1 = PartialTr42[ρ23] // Simplify
```

$$\left\{\left\{\frac{1}{2}(\alpha\,\alpha 1 + \beta\,\beta 1), 0\right\}, \left\{0, \frac{1}{2}(\alpha\,\alpha 1 + \beta\,\beta 1)\right\}\right\}$$