# Density Matrices

## 1 Abstract

Firstly our aim is to describe a N-body quantum system in both separable and inseparable states case,in both of them each subsystem's wave function lives in a d-dimensional Hilbert space $C^d$. Then we focus on case N=2 and we will test the program in case of two qubits with spin one-half.

## 2 Theory

Suppose we have a N-body quantum system composed by N particles and each subsystem's wave function $\psi$ lives in d-dimensional Hilbert space $C^d$.
So we want to compute total system's wave function $\Psi(\psi_1, \psi_2 ... \psi_N) \in C^{d^N}$.
In order to achieve this aim ,in most general case , we must use $d^N$ complex coefficients : one for each possible system's state $|\alpha_1\alpha_2....\alpha_N>$,where $\alpha_i$ is i-th subsystem's base composed by d eigenvectors.

$$\Psi = \sum_{\alpha_1,\alpha_2,...,\alpha_N} C_{\alpha_1,\alpha_2,...,\alpha_N} |\alpha_1\alpha_2...\alpha_N> \tag{1}$$

Nevertheless if $\Psi$ is composed by all *separable* states and so $|\alpha_1\alpha_2....\alpha_N> = |\alpha_1\rangle \otimes |\alpha_2\rangle \otimes \cdots \otimes |\alpha_N\rangle$ we need only $Nd$ complex coefficients and previous formula becomes:

$$\Psi = \bigotimes_{i=1}^{N} \sum_{\alpha_i} C_{i,\alpha_i} |\alpha_i\rangle \tag{2}$$

Then we can define *density matrix* as $\rho = |\Psi\rangle \langle\Psi|$ and also *reduced* ones for each subsystem .

## 3 Code development

My code is composed by two units program : one *module* and one *main program*.

- MODULE ***ex8***:

  here we define 3 functions and 1 subroutine :
  $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$ functions,receive ,as inputs, number of subsystems $N$,their Hilbert space dimension $d$ and,respectively, a complex coefficients list $coeff$ with $dN$ and $d^N$ elements.
  In this way we can compute and print on terminal total system's wave function $\Psi$ both in separable and inseparable case.
  For aesthetic reason $\boldsymbol{a}_2$ receives also, as input, a logical variable *bool* : if *bool* is TRUE the code will print total system's wave function as inseparable case otherwise it will print total system's wave function as separable one.
  In $\boldsymbol{b}$ function given (d,N,$\Psi$) , we compute ,the *density matrix* $\rho$ .
  In $\boldsymbol{c}$ subroutine given (d,$\rho$),we compute the *reduced matrices* $\rho_1$ and $\rho_2$ for subsystem 1 and 2 .

```
rho_1=(0.0,0.0)
rho_2=(0.0,0.0)

do k=1,d
       do h=1,d
              do i=1,d

                            rho_1(k,h)=rho_1(k,h)+rho( i+(k-1)*d, i+(h-1)*d )

              end do

       end do

end do

do k=1,d
       do h=1,d
              do i=1,d

                            rho_2(k,h)=rho_2(k,h)+rho( i+(i-1)*(d-1)+(k-1), i+(i-1)*(d-1)+(h-1) )

              end do

       end do

end do
```

- PROGRAM ***main***:

  here i recall module defined above and define two different complex coefficients list $n.i.states$ and $i.states$ that they will be passed as $coeff$ to $a_1$ and $a_2$ functions .
  Furthermore here define *bool* logical variable and its value .

## 4 Results

In order to test if program works properly,as suggest by exercise itself, we simulate a system composed by N=2 qubits ,$A$ and $B$, in d=2 possible spin states.
In separable case in order to visualize better subsystem's wave function we use $|0\rangle$ and $|1\rangle$ otherwise for inseparable one we use $|00\rangle$,$|01\rangle$,$|10\rangle$ and $|11\rangle$.

So we let begins showing separable case :

$$\Psi = \left( \frac{1}{\sqrt{2}} |0\rangle_A + \frac{1}{\sqrt{2}} |1\rangle_A \right) \otimes |0\rangle_B \tag{3}$$

```
Total wavefunction for  2 non interacting particles is :
(
(  0.7071068+ 0.0000000*i ) | 0>_particle 1+
(  0.7071068+ 0.0000000*i ) | 1>_particle 1+
)
(X)
(
(  1.0000000+ 0.0000000*i ) | 0>_particle 2+
(  0.0000000+ 0.0000000*i ) | 1>_particle 2+
)

 The density matrix is :

|          (0.499999970,0.00000000)          (0.00000000,0.00000000)          (0.499999970,0.00000000)          (0.00000000,0.00000000) |
|           (0.00000000,0.00000000)          (0.00000000,0.00000000)           (0.00000000,0.00000000)          (0.00000000,0.00000000) |
|          (0.499999970,0.00000000)          (0.00000000,0.00000000)          (0.499999970,0.00000000)          (0.00000000,0.00000000) |
|           (0.00000000,0.00000000)          (0.00000000,0.00000000)           (0.00000000,0.00000000)          (0.00000000,0.00000000) |

 The reduced density matrix for subsystem 1 is :

|          (0.499999970,0.00000000)          (0.499999970,0.00000000) |
|          (0.499999970,0.00000000)          (0.499999970,0.00000000) |

 The reduced density matrix for subsystem 2 is :

|          (0.999999940,0.00000000)          (0.00000000,0.00000000) |
|           (0.00000000,0.00000000)          (0.00000000,0.00000000) |
```

and then we continue with an example of inseparable one:

$$\Psi = \left( \frac{1}{\sqrt{2}} |00\rangle - \frac{1}{\sqrt{2}} |11\rangle \right) \tag{4}$$

```
Total wavefunction for  2 interacting particles is :

(  0.7071068+ 0.0000000*i )*|00>
+
(  0.0000000+ 0.0000000*i )*|01>
+
(  0.0000000+ 0.0000000*i )*|10>
+
( -0.7071068+ 0.0000000*i )*|11>

 The density matrix is :

|          (0.499999970,0.00000000)          (0.00000000,0.00000000)          (0.00000000,0.00000000)         (-0.499999970,0.00000000) |
|           (0.00000000,0.00000000)          (0.00000000,0.00000000)          (0.00000000,0.00000000)          (-0.00000000,0.00000000) |
|           (0.00000000,0.00000000)          (0.00000000,0.00000000)          (0.00000000,0.00000000)          (-0.00000000,0.00000000) |
|          (-0.499999970,0.00000000)         (-0.00000000,0.00000000)         (-0.00000000,0.00000000)         (0.499999970,-0.00000000) |

 The reduced density matrix for subsystem 1 is :

|          (0.499999970,0.00000000)          (0.00000000,0.00000000) |
|           (0.00000000,0.00000000)          (0.499999970,0.00000000) |

 The reduced density matrix for subsystem 2 is :

|          (0.499999970,0.00000000)          (0.00000000,0.00000000) |
|           (0.00000000,0.00000000)          (0.499999970,0.00000000) |
```

## 5 Comments and Self-Evaluation

Dealing with efficiency,from computational point of view,initialize separable states is more convenient than inseparable ones.
In fact ,starting from N=2 and d=2 (simplest case), $dN \leq d^N$ always for each couple $(N, d)$

Next upgrade can be to generalize reduced density matrices for generic N subsystems.