

Density Matrices

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- Quantum N-bodies system formed by N subsystems, each described $\psi_i \in \mathcal{H}^d$, is represented by $\Psi(\psi_1, \psi_2, \dots, \psi_N)$
 1. if ψ_i are non interacting, Ψ separable pure state: $d \cdot N$ coefficients (info is "compressed"!)
 2. general case $\Psi \in \mathcal{H}^{\otimes N}$: needed d^N coefficients
- Density matrix $\rho = \sum_{k=1}^N |\psi_k\rangle\langle\psi_k|$
 1. Hermitian
 2. $\text{Tr}(\rho) = 1$ if Ψ is normalized
 3. $\rho^2 = \rho$ if Ψ is pure, hence $\text{Tr}(\rho^2) = 1$ (ρ has been built as a projector)
- Reduced density matrix for subsystem B (i.e. tracing over A):
 1. $(\rho_B)_{mn} = \sum_i \langle i_A | \langle m_B | \rho | n_B \rangle | i_B \rangle$
 2. Hermitian
 3. $\text{Tr}(\rho_{red}) = 1$
 4. Purity is not conserved anymore! $\text{Tr}(\rho_{red}^2) \neq 1$

$\Psi_{\text{separable}} \rightarrow \Psi_{\text{FULL}}$.

Mapping similar to change of basis $Num_{10} \rightarrow Num_d$ with N digits.

```
1 DO jj = 1, psi_multi_state%n_vectors
2   rest = MOD(temp, psi_multi_state%d_dim)
3   index_separable = 1+rest+(psi_multi_state%n_vectors-
4     jj)*psi_multi_state%d_dim
5   psi_multi_state%coeffs(ii+1) = &
6     & psi_multi_state%coeffs(ii+1)*psi_separable%coeffs(
7     index_separable)
8   temp = (temp-rest)/psi_multi_state%d_dim
9 END DO
```

Given Ψ , to compute ρ :

```
1 FUNCTION OUTER_PROD_vec(x,y) RESULT(res)
2   TYPE(CMATRIX) :: res; COMPLEX*16, DIMENSION(:) :: x,y
3   res%dims(1) = SIZE(x); res%dims(2) = SIZE(y)
4   res%element = MATMUL(RESHAPE(x, (/res%dims(1),1/)),
5     RESHAPE(CONJG(y), (/1,res%dims(2)/)))
6 END FUNCTION
```

- Computational limits (How large N can be?)
 1. Given by memory storage, specially for the matrix
 2. Double complex variable occupies 16 bytes
 3. 5-6 GB RAM usually free, thus $d^{2N} \lesssim 4 \cdot 10^8$
 4. if qubits ($d = 2$), $N_{max} = 14$ ($\sim 4.3GB$).
As other examples ($d = 3, N = 9$) or ($d = 5, N = 7$) are already too much!
- Debug
 1. Parameters are meaningful ($d, N > 0$)
 2. Size of vectors compatible if coefficients, separable flag, number of subsystems N and d were given (either $d \cdot N$ or d^N)
 3. If $\Psi_{separable}$, first need compute Ψ_{full} and then ρ
 4. ρ is Hermitian
 5. $Tr(\rho) = 1$
 6. $\rho^2 = \rho$
 7. ρ_{red} is Hermitian
 8. $Tr(\rho_{red}) = 1$

Bell State

$$\text{Bell state } |\psi^-\rangle = \frac{1}{\sqrt{2}} (|01\rangle - |10\rangle)$$

What we expect:

$$\rho_{12} = \frac{1}{2} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

$$\rho_1 = \rho_2 = \frac{1}{2} \mathbb{1}_2$$

Results

Density matrix:

```
( 0.00E+00, 0.00E+00) ( 0.00E+00, 0.00E+00) ( 0.00E+00, 0.00E+00) ( 0.00E+00, 0.00E+00)
( 0.00E+00, 0.00E+00) ( 5.00E-01, 0.00E+00) (-5.00E-01, 0.00E+00) ( 0.00E+00, 0.00E+00)
( 0.00E+00, 0.00E+00) (-5.00E-01, 0.00E+00) ( 5.00E-01, 0.00E+00) ( 0.00E+00, 0.00E+00)
( 0.00E+00, 0.00E+00) ( 0.00E+00, 0.00E+00) ( 0.00E+00, 0.00E+00) ( 0.00E+00, 0.00E+00)
```

Reduced density matrix tracing over subsystem 1:

```
( 5.00E-01, 0.00E+00) ( 0.00E+00, 0.00E+00)
( 0.00E+00, 0.00E+00) ( 5.00E-01, 0.00E+00)
```

Reduced density matrix tracing over subsystem 2:

```
( 5.00E-01, 0.00E+00) ( 0.00E+00, 0.00E+00)
( 0.00E+00, 0.00E+00) ( 5.00E-01, 0.00E+00)
```

Further developments

- Dealing better with inputs and, more advanced, mixed states
- Check for non-negativeness of density matrix