Density Matrices

Andrea Nicolai

Università degli Studi di Padova

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Theory

- Quantum N-bodies system formed by N non entangled subsystems, each described $\psi_i \in \mathcal{H}^d$, is represented by $\Psi(\psi_1, \psi_2, ...\psi_N)$
  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. $Tr(\rho) = 1$ if Ψ is normalized
  3. $\rho^2 = \rho$ if Ψ is pure, hence $Tr(\rho^2) = 1$ (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. $Tr(\rho_{red}) = 1$
  4. Purity is not conserved anymore! $Tr(\rho_{red}^2) \neq 1$

Code Development $\Psi(\psi_1, ...\psi_N)$ and density matrices

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

```
DO jj = 1, psi_multi_state%n_vectors
    rest = MOD(temp, psi_multi_state%d_dim)
    index_separable = 1+rest+(psi_multi_state%n_vectors-jj)*psi_multi_state%d_dim
    psi_multi_state%coeffs(ii+1) = &
    & psi_multi_state%coeffs(ii+1)*psi_separable%coeffs(index_separable)
    temp = (temp-rest)/psi_multi_state%d_dim
END DO
```

Given Ψ, to compute ρ:

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

Code Development Computational limits and Debug

- 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 $(d = 2)$, $N_{max} = 14$ $(\sim 4.3 GB)$.
     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

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

What we expect:

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

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

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