Density Matrices and N-bodies wave function

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- $\Psi \in H^{d^N}$ be a pure quantum state of a composite system and let $\{H_i^d\}$ be the set of N Hilbert spaces with basis $|n_i\rangle_{n=0}^{d-1}$ where the N subsystems composing it live.

$$|\Psi\rangle = \sum_{\{n_i\}} c_{\{n_i\}} \bigotimes_{n_i \in \{n_i\}} |n_i\rangle \qquad d^N \text{ coefficients} \tag{1}$$

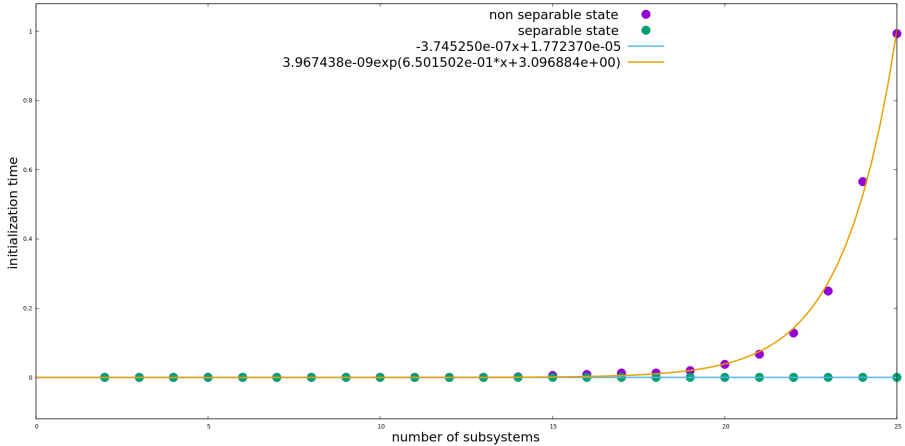
- Ψ is separable if it can take the following form.

$$|\Psi\rangle = \bigotimes_{i=1}^{N} |\psi_i\rangle \qquad d \times N \text{ coefficients} \tag{2}$$

Separable and Non-Separable Systems

Initialization Time

- Separable state $\longrightarrow N \times d$ complex*16 matrix.
- Non-separable $\longrightarrow d^N \times 1$ complex*16 matrix.



Code Approach

Types

To handle efficiently wave functions and density matrices of composite systems I defined two types.

```
type compositewf
    integer ::number
    integer ::states
    integer :: nclassicalmixture
    real*8, dimension(:),
        allocatable :: probs
    complex*16, dimension(:,:),
        allocatable :: wave
end type
```

```
type dnsmat
    integer ::nobodies
    integer :: nostatesxb
    double complex,
        dimension(:,:),
        allocatable :: mat
end type
```

Code Approach for Multi-Bodies Wave Function and Density Matrix

Functions

- **MergeWf** : from a complex*16 matrix (rows subsystem states, columns subsystems) computes a *compositewf* object for a pure state.

$$|\Psi\rangle = \bigotimes_{i=1}^{N} |\psi_i\rangle$$

- **BDMmb** : from a *compositewf* object (wavefunction + info) computes the respective *dnsmat* object.

$$\rho = |\Psi\rangle\langle\Psi|$$

- **marginalizeDMMB2** : from a *dnsmat* object and an array of integers (contains the index of the subsystems to keep) computes the reduced density matrix.

$$\rho_X = Tr_Y \rho$$

Reliability test

- Generate random wave functions for N subsystems $\left(\vec{\psi}_1 \quad \vec{\psi}_2 \quad ... \quad \vec{\psi}_N\right)$
- Use **MergeWf** to compute the total wave function of the system .

$$|\Psi\rangle = \bigotimes_{i=1}^{N} |\psi_i\rangle$$

- Compute the density matrix with **BDMmb** $\rho = |\Psi\rangle\langle\Psi|$
- Compute the reduced density matrix of one subsystem with **marginalizeDMMB2**

$$\rho_{\psi_i} = Tr_{\substack{\{\psi_j\} \\ j \neq i}} \rho$$

- Compare the output of the last passage with the density matrix computed directly

$$\rho_{\psi_i} \stackrel{?}{=} |\psi_i\rangle\langle\psi_i|$$

Reliability Test

This test have been done with 3 subsystems $\in H^3$.
The following pictures shows ρ_{ψ_i}.

```
------ Control density Matrix --------                 ------- Obtained density Matrix --------
 0.47  +0.00 i     0.10  -0.04 i     0.15  -0.46 i       0.47  -0.00 i     0.10  -0.04 i     0.15  -0.46 i
 0.10  +0.04 i     0.03  +0.00 i     0.08  -0.09 i       0.10  +0.04 i     0.03  -0.00 i     0.08  -0.09 i
 0.15  +0.46 i     0.08  +0.09 i     0.51  -0.00 i       0.15  +0.46 i     0.08  +0.09 i     0.51  -0.00 i
```

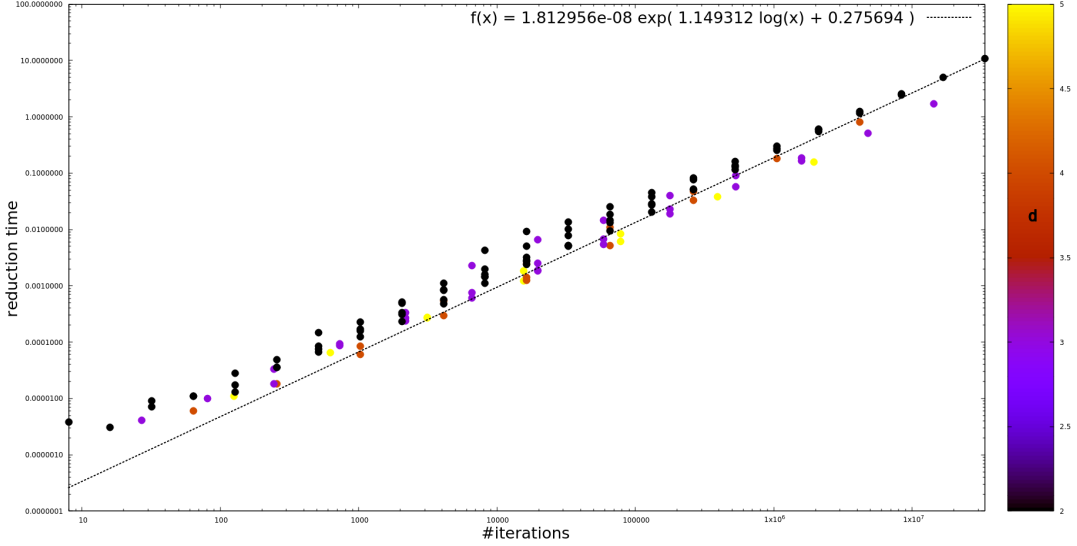
MarginalizeDMMB2 scaling time

Finally I focused on the scaling time of **MarginalizeDMMB2** function. This depends on three parameters:

- N = number of subsystems
- N^* = number of subsystems left out from the marginalization
- d = dimension Hilbert space subsystem

I decided to plot the computational time as function of the number of iteration derived from three nested **do loop** inside the function $\#iteration = d^{N+N^*}$

MarginalizeDMMB2 scaling time



Thanks for the attention