EXERCISE 6
DENSITY MATRICES FORMALISM

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EXERCISE GOALS

- Consider a quantum system formed by N subsystems (spins, atoms, particles etc..) each described by its wave function $\psi_i \in \mathcal{H}^D$ where $\mathcal{H}^D$ is a D-dimensional Hilbert space.
- Write a Fortran code to describe such a system (N-body non interacting, separable pure state) and a general N-body pure wave function $\psi \in \mathcal{H}^{D^N}$, commenting their efficiency.
- Given N = 2, write the density matrix of a pure state ψ, $\rho = |\psi><\psi|$
- Given a generic density matrix in $\mathcal{H}^{D^2}$ compute the reduce density matrix of either the left or the right system, e.g. $\rho_1 = Tr_2\ \rho$.
- Test the functions described before (and all others needed) on two-spin one-half (qubits) with different states.

IN THEORY…

- Many-body quantum state: $|\alpha_1 > \otimes |\alpha_2 > \otimes (\dots) \otimes |\alpha_N > \equiv |\alpha_1 \alpha_2 \dots \alpha_N >$
- Since $\alpha_i = 0,1, \dots D-1$, integer notation: $x = \alpha_1 D^{N-1} + (\dots) + \alpha_{N-1} D + \alpha_N$
- For a bipartite system $|\alpha\beta >$:

  $(\rho_A)_{ij} = (Tr_B \rho)_{ij} = \Sigma_\beta < \alpha_i \beta |\rho| \alpha_j \beta >$ where $|\alpha_j \beta > = |\alpha_j D + \beta >, \beta = 0, \dots \mathrm{D} - 1$

  $(\rho_B)_{ij} = (Tr_A \rho)_{ij} = \Sigma_\alpha < \alpha \beta_i |\rho| \alpha \beta_j >$ where $|\alpha \beta_j > = |\alpha D + \beta_j >, \alpha = 0, \dots \mathrm{D} - 1$

  Therefore, easy access to ρ elements according to integer index to sum onto
- To define a generic many-body quantum state: need to specify all the density matrix: $O(D^N)$
- To define a separable state: need D coefficients per subsystem (total $O(DN)$)

CODE DEVELOPMENT: ρ

Note: variable D ≡ D^N

- Define ρ as projector of pure state (outer product of ψ^*, ψ)
- Check purity: $Tr(\rho) = Tr(\rho^2) = 1$

```
function NewDensityMatrix(D) result(rho)
! Randomly initialize a DM for PURE STATE

    integer :: D
    double complex, dimension(D) :: psi
    double complex, dimension(D,D) :: rho

    psi = ComplexRandom(D)
    psi = psi/cnorm(psi,1.D0)
    rho = OuterProduct(conjg(psi),psi)

end function
```

```
Trace of Rho: (expected 1)
Type COMPLEX(8):                    (1.0000000000000000,0.0000000000000000)
Trace of Rho^2: (expected 1)
Type COMPLEX(8):           (0.99999999999999978,1.8847228466777379E-019)
```

*up to 100, time ≈ $5s$

CODE DEVELOPMENT: REDUCED ρ, N=2, LARGE D*

```
mel = 0.d0

do ii = 0, subsys_dim-1
    bra_idx = mm * subsys_dim**system_rank + ii * subsys_dim**(1-system_rank) + 1
    ket_idx = nn * subsys_dim**system_rank + ii * subsys_dim**(1-system_rank) + 1
    mel = mel + rho_AB(bra_idx,ket_idx)
end do
```

- Generate random density matrix for whole system
- Update each reduced density matrix element summing al suitable indexes
- Check on reduced ρ: expected unitary trace
- In general, non-pure states: $Tr(\rho^2) \neq 1$
- Try for different values of size for system

```
Trace of Rho_A:
Type COMPLEX(8):                (1.0000000000000002,0.0000000000000000)
Trace of Rho_A^2:
Type COMPLEX(8):          (0.22299328685022135,-4.5005841519304140E-019)
Trace of Rho_B:
Type COMPLEX(8):                (1.0000000000000004,0.0000000000000000)
Trace of Rho_B^2:
Type COMPLEX(8):          (0.22299328685022132,7.9393730230824319E-020)
```

CODE DEVELOPMENT: KNOWN QUBIT STATES

PURE, SEPARABLE STATE:

$$|\psi>_{AB} = |00>_{AB}$$

```
! Test for AB state: |00>

psi = 0.d0
psi(1) = complex(1,0)
rho = OuterProduct(conjg(psi),psi)
```

Expected pure state

```
 ---------- AB in | 00 > ----------
 rho_A:
(  1.00  +0.00 i) (  0.00  +0.00 i)
(  0.00  +0.00 i) (  0.00  +0.00 i)
 rho_B:
(  1.00  +0.00 i) (  0.00  +0.00 i)
(  0.00  +0.00 i) (  0.00  +0.00 i)
```

PURE, MAXIMALLY ENTANGLED STATE:

$$|\psi>_{AB} = {}^{1}/_{\sqrt{2}}(|00>_{AB} + |11>_{AB})$$

```
! Test for AB state: |psi+> (Bell state)

rho = 0.d0
rho(1,1) = 1./2.
rho(1,4) = 1./2.
rho(4,1) = 1./2.
rho(4,4) = 1./2.
```

Expected maximally mixed state

```
 ---------- AB in |psi + > ----------
 rho_A:
(  0.50  +0.00 i) (  0.00  +0.00 i)
(  0.00  +0.00 i) (  0.50  +0.00 i)
 rho_B:
(  0.50  +0.00 i) (  0.00  +0.00 i)
(  0.00  +0.00 i) (  0.50  +0.00 i)
```