Quantum information and computing: Exercises report, week 4. Multi-run script & Automated fits

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Through the exercise of this week, we start to tackle the Many-Body Problem. We will try to implement some methods to handle N-body non interacting, separable/non-separable, pure states. We will write the density matrix of a pure state given $N = 2$, exploit a subroutine to compute the reduce density matrix of either the left or the right subsystem once a density matrix in $\mathcal{H}^{D^2}$ is given. Finally, we will test all the instruments deleveloped on a system made of two qubits.

I. THEORY

Considering a system made of N particles, each one described by a wavefunction ψ_i living in a d-dimensional Hilbert space $\mathcal{H}^d$, we have that the wavefunction Ψ of the whole system is given by:

$$|\Psi\rangle = \sum_{\alpha_1,\dots,\alpha_N} C_{\alpha_1,\dots,\alpha_N} |\psi_{\alpha_1}\rangle \otimes |\psi_{\alpha_2}\rangle \otimes \cdots \otimes |\psi_{\alpha_N}\rangle \qquad \alpha_j \in \{1,\dots,D\} \tag{1}$$

Sometimes we encounter special kind of states, called separable, which can be written as a sum of N pure state over each subsystem. In other words, we call a state separable if we can write it as:

$$|\Psi\rangle = \sum_{\alpha_1} C_{\alpha_1} |\psi_{\alpha_1}\rangle \otimes \sum_{\alpha_2} C_{\alpha_2} |\psi_{\alpha_2}\rangle \otimes \cdots \otimes \sum_{\alpha_N} C_{\alpha_N} |\psi_{\alpha_N}\rangle \tag{2}$$

and so describe it with only dN coefficients instead of d^N.
Given a generic state $|\Psi\rangle$ the density matrix ρ that describes that state is defined as:

$$\rho = |\Psi\rangle\langle\Psi| \tag{3}$$

Describing a quantum state by its density matrix is a fully general alternative formalism to describing a quantum state by its state vector (its "ket") or by a statistical ensemble of kets Given a generic density matrix ρ in $\mathcal{H}^{d^N}$, the reduced density matrix relative to the k-subsystem is:

$$\rho_k = Tr_1 \dots Tr_{k-1} Tr_{k+1} \dots Tr_N \rho \qquad \text{where} \qquad \mathrm{Tr}_j\, \rho = \sum_{j=1}^{D} \langle j|\, \rho\, |j\rangle \tag{4}$$

II. CODE DEVELOPMENT

In order to describe properly any kind of state separable or not I implemented a derived type in fortran called *pure_state*

```fortran
type pure_state
  integer(kind=8) :: dim
  integer(kind=8) :: N_particles
  logical :: is_separable
  complex(kind=8), dimension(:), allocatable :: psi
end type
```

where it is initialized the dimension of any subsystem, the number of particles our system is made of, a logical variable that controls if the state is separable or not, and a complex arrays that has to be properly initialized to describe the state. Moreover, I implemented a subroutine useful to allocate properly the memory based on the kind of the state:

```fortran
!!!!!!!!!!!!!!!!!!! allocate the memory for a pure state !!!!!!!!!!!!!!!!!!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!! separable or not !!!!!!!!!!!!!!!!!!!!!!!!!!!!!
subroutine init_pure_state(state,dim,N,separable)
  type(pure_state) :: state
  integer(kind=8) :: dim
  integer(kind=8) :: N
  logical :: separable

  if ( separable ) then
    state%dim = dim
    state%N_particles = N
    allocate(state%psi(dim*N))
    state%is_separable = .true.
  else
    state%dim = dim
    state%N_particles = N
    allocate(state%psi(dim**N))
    state%is_separable = .false.
  end if
end subroutine init_pure_state
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
```

where if the state is separable, then the dimension of the array is given by dN, otherwise it will be d^N. Therefore, I implemented some subroutine to per form operations on complex arrays and matrices:

```
!!!!!!!!!!!!!!!!!! compute the trace of a cmplx matrix !!!!!!!!!!!!!!!!!!
  subroutine trace(matrix, tr)
    complex(kind=8), dimension(:,:), intent(in) :: matrix
    complex(kind=8) :: tr
    integer, dimension(2) :: dimm
    integer :: ii
    dimm = shape(matrix)
    do ii=1, dimm(1)
        tr = tr + matrix(ii,ii)
    end do
  end subroutine trace
  !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!


  !!!!!!!!!!!!!!!!!!! outer product of two complex arrays !!!!!!!!!!!!!!!!!!
  subroutine dyadics(x,y,mat)
    complex(kind=8), dimension(:) :: x,y
    complex(kind=8), dimension(:,:), allocatable :: mat
    integer :: nn, mm
    nn = size(x)
    mm = size(y)
    mat = matmul(reshape(x, (/nn,1/)), reshape(conjg(y), (/1,mm/)))
  end subroutine dyadics
  !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

  !!!!!!!!!!!!!!!!! tensor product of two complex matrices !!!!!!!!!!!!!!!!
  subroutine tensor_product(mat_1, mat_2, mat_prod)
      complex(kind=8), dimension(:,:):: mat_1, mat_2
      complex(kind=8), dimension(:, :), allocatable :: mat_prod
      integer :: ii, jj
      integer, dimension(2) :: dimm_1, dimm_2

      dimm_1 = shape(mat_1)
      dimm_2 = shape(mat_2)

      allocate (mat_prod(dimm_1(1)*dimm_2(1), dimm_1(1)*dimm_2(1)))
      do ii=1, dimm_1(1)
          do jj=1, dimm_1(1)
```

```
              mat_prod((ii-1)*dimm_2(1)+1:ii*dimm_2(1),&
              (jj-1)*dimm_2(1)+1:jj*dimm_2(1))=mat_1(ii,jj)*mat_2
          end do
      end do
    end subroutine tensor_product
  !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
```

In particular, the three subroutines above computes the trace, implements the dyadics operation on two complex arrays and the tensor product between two complex matrices.
Finally, I implemented these two subroutines to compute the right and left partial trace on a system of two qbits or, in more general terms, on a bipartite matrix:

```
!!!!!!!!!!!!!!!!!!! compute the left partial trace !!!!!!!!!!!!!!!!!!!
!!!!!!!!!!!!!!!!!!!!!! for a bi-partite matrix !!!!!!!!!!!!!!!!!!!!!!
subroutine partial_trace_a_he(rho, da, db, rho_b)
integer(kind=4) :: da, db
complex(kind=8), dimension(:,:) :: rho
complex(kind=8), dimension(:,:), allocatable :: rho_b
integer :: j, k, l  ! Auxiliary variable for counters

allocate(rho_b(db,db))

rho_b = 0.d0

do j = 1, db
  do k = j, db
    do l = 1, da
      rho_b(j,k) = rho_b(j,k) + rho((l-1)*db+j,(l-1)*db+k)
    end do
    if ( j .ne. k ) then
      rho_b(k,j) = conjg(rho_b(j,k))
    end if
  end do
end do
end subroutine partial_trace_a_he
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!



!!!!!!!!!!!!!!!!!!! compute the right partial trace !!!!!!!!!!!!!!!!!!
!!!!!!!!!!!!!!!!!!!!!! for a bi-partite matrix !!!!!!!!!!!!!!!!!!!!!!
subroutine partial_trace_b_he(rho, da, db, rho_a)
implicit none
integer(kind=4), intent(in) :: da, db
complex(kind=8), dimension(:,:) :: rho
complex(kind=8), dimension(:,:), allocatable :: rho_a
integer :: j, k, l  ! Auxiliary variables for counters

allocate(rho_a(db,db))

rho_a = 0.d0
do j = 1, da
  do k = j, da
    do l = 1, db
      rho_a(j,k) = rho_a(j,k) + rho((j-1)*db+l,(k-1)*db+l)
    end do
    if ( j .ne. k ) then
      rho_a(k,j) = conjg(rho_a(j,k))
    end if
  end do
end do
end subroutine partial_trace_b_he
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
```

III. RESULTS

Here, I test the previously shown routines to exploit the property of a two qbits system in a given state:

```
program qbits
use ex08module
implicit none

type(pure_state) :: state
integer(kind=8) :: dim, N
logical :: separable
complex(kind=8), dimension(:,:), allocatable :: rho, rho_a, rho_b
real(kind=8) :: norm

dim = 2
N = 2
separable = .true.
norm = 2


call init_pure_state(state,dim,N,separable)

state%psi(1) = cmplx(1/sqrt(norm),0)
state%psi(2) = 0
state%psi(3) = 0
state%psi(4) = cmplx(-1/sqrt(norm),0)

call dyadics(state%psi,state%psi,rho)
call partial_trace_a_he(rho, 2, 2, rho_b)
call partial_trace_b_he(rho, 2, 2, rho_a)


call write_a_complex_matrix('psi',rho)
call write_a_complex_matrix('rho_reduced_over_a',rho_b)
call write_a_complex_matrix('rho_reduced_over_b',rho_a)

end program qbits
```

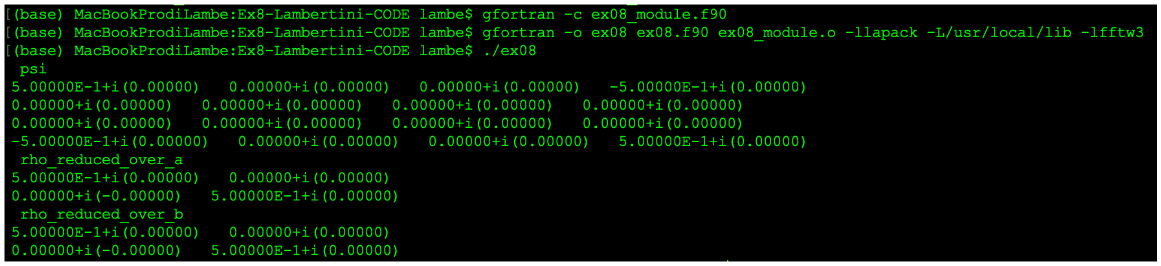
The state tested here is:

$$|\Psi\rangle = \frac{1}{\sqrt{2}}|00\rangle - \frac{1}{\sqrt{2}}|11\rangle$$

which is described by the density matrix:

$$\rho = \begin{bmatrix} \frac{1}{\sqrt{2}} \\ 0 \\ 0 \\ -\frac{1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{2}} & 0 & 0 & -\frac{1}{\sqrt{2}} \end{bmatrix} = \begin{bmatrix} \frac{1}{2} & 0 & 0 & -\frac{1}{2} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -\frac{1}{2} & 0 & 0 & \frac{1}{2} \end{bmatrix} \tag{5}$$

Below I show the results obtained by running the above program:



```
[(base) MacBookProdiLambe:Ex8-Lambertini-CODE lambe$ gfortran -c ex08_module.f90
[(base) MacBookProdiLambe:Ex8-Lambertini-CODE lambe$ gfortran -o ex08 ex08.f90 ex08_module.o -llapack -L/usr/local/lib -lfftw3
[(base) MacBookProdiLambe:Ex8-Lambertini-CODE lambe$ ./ex08
 psi
5.00000E-1+i(0.00000)   0.00000+i(0.00000)   0.00000+i(0.00000)   -5.00000E-1+i(0.00000)
0.00000+i(0.00000)   0.00000+i(0.00000)   0.00000+i(0.00000)   0.00000+i(0.00000)
0.00000+i(0.00000)   0.00000+i(0.00000)   0.00000+i(0.00000)   0.00000+i(0.00000)
-5.00000E-1+i(0.00000)   0.00000+i(0.00000)   0.00000+i(0.00000)   5.00000E-1+i(0.00000)
 rho_reduced_over_a
5.00000E-1+i(0.00000)   0.00000+i(0.00000)
0.00000+i(-0.00000)   5.00000E-1+i(0.00000)
 rho_reduced_over_b
5.00000E-1+i(0.00000)   0.00000+i(0.00000)
0.00000+i(-0.00000)   5.00000E-1+i(0.00000)
```

FIG. 1. Output of the program *ex08.f90*

We can see that the results are coherent with what expected from theory.

IV. SELF-EVALUATION

I think the main objectives of the exercise are reached. I have learnt how to implement tensor operations in Fortran in the quantum-mechanical framework. I'm aware that the report is not rich enough of details and explanations but I have not had much time this week, I hope that the work is still sufficient.