

# Name: Yifan Tian ID: 78921267

1.

(a)

```
function normsq1(A)
    l = size(A)[1]
    (m1,n,m2) = size(A[1])
    mpsl = zeros(m1,m1,m2,m2)
    for u1 = 1:m1, d1 = 1:m1, s = 1:n, mu1= 1:m2, md1 = 1:m2
        mpsl[u1,d1,mu1,md1] += A[1][u1,s,mu1]*A[1][d1,s,md1]
    end
    for i = 2:l
        mpsr = zeros(m1,m1,m2,m2)                                     #key difference with tensor
        contraction, not herit.
        for u1 = 1:m1, d1 = 1:m1, s = 1:n, mu1= 1:m2, md1 = 1:m2, mui = 1:m2, mdi = 1:m2
            mpsr[u1,mui,mdi,d1] += mpsl[u1,mu1,md1,d1]*A[i][mu1,s,mui]*A[i][mdi,s,mdi]
        end
        mpsl = mpsr
    end
    return mpsl[1,1,1,1]
end
normsq1(A) = 1
```

(b)

```
function normsq2(A)
    l = size(A)[1]
    (m1,n,m2) = size(A[2])
    mps1 = reshape(A[1],m1*m2,n)*reshape(A[1],n,m1*m2)                # put the contraction side
    together.
    mps1 = reshape(mps1,m1*m1*m2,m2)
    for i = 2:l
        mps1d = mps1*reshape(A[i],m1,n*m2)
        mps2 = reshape(mps1d,m2,n*m1)*reshape(A[i],n*m1,m2)
        mps1 = reshape(mps2,m1,m1)
    end
    return mps1[1,1,1,1]
end
normsq2(A) = 1
```

(c)

```
function normsq3(A)
    l = length(A)
    A1 = A[1]
    @tensor begin
        mpsl[u1,d1,mu1,md1] := A1[u1,s,mu1]*A1[d1,s,md1]
    end
    for i = 2:l
```

```

    A1 = A[i]
    @tensor mpsl[u1,d1,mu1,md1] = mpsl[u1,d1,mu,md]*A1[mu,s,mu1]*A1[md,s,md1]
end
return mpsl[1,1,1,1]
end
normsq3(A) = 1

```

## 2.

```

type MPS
    A
    oc::Int64
end
mp = MPS(A,1)

```

move OC:

One tricky part: when do from right to left. The QR(A[n,m]) in julia always decompose in Q\*R based on the order of argument in the function.

```

function moveto!(psi::MPS,i::Int64)
    if i > psi.oc
        # move OC from left
    to right
        for n = psi.oc:i-1
            (ml,s,mr) = size(psi.A[n])
            intmps = reshape(psi.A[n],ml*s,mr)
            intq = qr(intmps)[1]; intr = qr(intmps)[2]
            # do QR decomposition
        if ml*s >= mr
            psi.A[n] = reshape(intq,ml,s,mr)
            # from Q to construct
        left tensor
        else
            psi.A[n] = reshape(intq,ml,s,ml*s)
        end
        (ml_r,s_r,mr_r) = size(psi.A[n+1])
        if ml*s >= ml_r
            psi.A[n+1] = reshape(intr*reshape(psi.A[n+1],ml_r,s_r*mr_r),ml_r,s_r,mr_r)
            # multiply
        right site with R
        else
            psi.A[n+1] = reshape(intr*reshape(psi.A[n+1],ml_r,s_r*mr_r),ml*s,s_r,mr_r)
        end
        end
    elseif i < psi.oc
        # move OC from
    right to left
        for n = psi.oc:-1:(i+1)
            (ml,s,mr) = size(psi.A[n])
            intmps = reshape(psi.A[n],mr*s,ml)
            intq = qr(intmps)[1]; intr = qr(intmps)[2]
            #tricky part
        if mr*s >= ml
            psi.A[n] = reshape(transpose(intq),ml,s,mr)
            #transpose to keep right order of indices
        end
        end
    end
end

```

```

else
  psi.A[n] = reshape(transpose(intq),mr*s,s,mr)
end
(ml_l,s_l,mr_l) = size(psi.A[n-1])
if mr*s > mr_l
  psi.A[n-1] = reshape(reshape(psi.A[n-1],ml_l*s_l,mr_l)*intr,ml_l,s_l,mr_l)
else
  psi.A[n-1] = reshape(reshape(psi.A[n-1],ml_l*s_l,mr_l)*intr,ml_l,s_l,mr*s)
end
end
end
psi.oc = i
return psi
end

```

### 3.

**Idea of energybond program: move oc to the gauge position. use the feature of OC (orthogonality) to measure the operator.**

```

function energybond(psi::MPS,i::Int64)
  l = size(psi.A)[1]
  psi = moveto!(psi,i)
  mptwo1 = psi.A[i]; mptwo2 = psi.A[i+1]
  @tensor begin
    szbond = scalar(mptwo1[m1,usz1,eu]*mptwo2[eu,usz2,m2]*Htwosite[usz1,usz2,dsz1,dsz2]*mpt-
    wo1[m1,dsz1,ed]*mptwo2[ed,dsz2,m2])
  end
  return szbond
end

```

when we have energybond program, we can use the summation to calculate the energy of the system.

```

function energy_oc(psi::MPS)
  #calculate heisenberg energy using energybond
  l = size(psi.A)[1]
  energy = 0
  for i = 1:l-1
    energy += energybond(psi,i)
  end
  mp_norm = normsq3(psi)
  return energy/mp_norm
end

```

for product state A. the energybond is -0.25

energybond(A) = -0.25

The energy of a n-site product state is 0.25(n-1).

## 4. The idea of imaginary time evolution:

```
function TEBD(psi::MPS,nt,m)
```

```
l = size(psi.A)[1]
```

```
for t = 1:nt
```

#  $nt = \frac{\beta}{\tau}$ , number of sweep

```
    psi = sweep(psi,m)
```

```
    newpsi = tensor_reverse(psi)
```

```
    newpsi = sweep(newpsi,m)
```

```
    psi = tensor_reverse(newpsi)
```

```
end
```

```
return psi
```

```
end
```

```
function tensor_reverse(psi::MPS)
```

#reverse the tensor to use dosvdtoright()

```
twice.
```

```
l = size(psi.A)[1]
```

```
newpsiA = 0*psi.A
```

```
for i = l:-1:1
```

```
    psiAi = psi.A[i]
```

```
    (a,b,c) = size(psiAi)
```

```
    tensor_i = zeros(c,b,a)
```

```
    @tensor tensor_i[c,b,a] = psiAi[a,b,c]
```

```
    newpsiA[l-i+1] = tensor_i
```

```
end
```

```
newoc = l-psi.oc+1
```

```
return MPS(newpsiA,newoc)
```

```
end
```

```
function sweep(psi::MPS,m)
```

//sweep from head to tail.

```
l = size(psi.A)[1]
```

```
for i = 1:l-1
```

```
    Ai = psi.A[i]
```

```
    Ai1 = psi.A[i+1]
```

```
    @tensor begin
```

```
        AA[a,f,g,e] := Ai[a,b,c]*Ai1[c,d,e]*taugate[b,d,f,g]
```

```
    end
```

```
    (psi.A[i],psi.A[i+1])=dosvdtoright(AA,m)
```

```
end
```

```
psi.oc = l
```

```
return psi
```

```
end
```

```
function dosvdtoright(AA,m::Int64)
```

```
(a,b,c,d) = size(AA)
```

```
AA = reshape(AA,a*b,c*d)
```

```
mpsl = svd(AA)[1]
```

```
spectrum = svd(AA)[2]
```

```

right = svd(AA)[3]
D = zeros(m,m)
Dm = length(spectrum)
if Dm > m                                     #do truncation
  [D[i,i] = spectrum[i] for i = 1:m]
  right = D*transpose(right[:,1:m])
  return (reshape(mpsl[:,1:m],a,b,m), reshape(right,m,c,d))
else                                           #grow to the truncation cut-off m.
  [D[i,i] = spectrum[i] for i = 1:Dm]
  right = D[1:Dm,1:Dm]*transpose(right[:,1:Dm])
  return (reshape(mpsl[:,1:Dm],a,b,Dm), reshape(right,Dm,c,d))
end
end
end

```

Plot of the time-evolution of 20-sites,  $\beta = 1$ ,  $\tau = 0.01$ .  $nstep = \frac{\beta}{\tau} = 100$

