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## Tutorial 03\_jl: SVD, MPO, Fermions

### Solution T03.1: Reshaping a general tensor into MPS form [6]

#### (a) SVD a tensor without or with truncation

(i) *Write your own SVD function.* There is a new function `svdTr` under the `Tensor` directory. Compare this with your version.

**Note:** `svdTr` returns  $V^\dagger$  while `svd` returns  $V$ . Also, `svdTr` returns  $S$  as a vector while `svd` returns  $S$  as either a matrix or a vector depending on a setting.

(ii) *Test your code.* We test `svdTr` for the GHZ state as follows.

```
1 using LinearAlgebra
2 using Printf
3
4 include("Tensor.jl")
5
6 ## Perform an SVD on the GHZ state
7 GHZ3 = zeros(2,2,2); #[s1]x[s2]x[s3]
8 GHZ3[1,1,1] = 1/sqrt(2); # |000>
9 GHZ3[2,2,2] = 1/sqrt(2); # |111>
10 ## (1)
11 U,S,Vd = svdTr(GHZ3,3,1,Inf,0)
12 ## (2)
13 # Verify U S V^\dagger = T_GHZ
14 T_GHZ = contract(U,2,1,contract(diagm(S),2,1,Vd,3,1),3,1)
15 err = sum(GHZ3-T_GHZ)
16 @printf("SVD error: %.4f %%\n",err)
17 # Verify S = Diagonal([1, 1]) / \sqrt(2)
18 S
19 ## (3)
20 # Set NKeep = 1
21 _,_,_,dw = svdTr(GHZ3,3,1,1,0)
22 dw # Discarded weight = 0.5
23 ## (4)
24 U,S,Vd = svdTr(GHZ3,3,[1,2],Inf,0)
25 size(U) # rank-3 tensor
26 size(S) # S is a vector
27 size(Vd) # rank-2 tensor [matrix]
28 # Verify U S V^\dagger = T_GHZ
29 T_GHZ = contract(U,3,3,contract(diagm(S),2,1,Vd,2,1),2,1)
30 err = sum(GHZ3-T_GHZ)
31 @printf("SVD error: %.4f %%\n",err)
32 # Verify S = Diagonal([1, 1]) / \sqrt(2)
33 S
```

#### (b) Write a GHZN state as an MPS

[i]  $N = 2$ . The tensor network diagram for an SVD representation of  $|\text{GHZ2}\rangle$  is

$$|\text{GHZ2}\rangle = \left(|0\rangle_1 \quad |1\rangle_1\right) \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} |0\rangle_2 \\ |1\rangle_2 \end{pmatrix} =: \mathcal{A} \Lambda \mathcal{B} =: |\sigma_1\rangle_1 A^{\sigma_1} \Lambda |\sigma_2\rangle_2 B^{\sigma_2} = \star \underset{\sigma_1}{\underset{1}{\downarrow}} \alpha \quad \bigcirc \quad \underset{\beta}{\underset{1}{\downarrow}} \star.$$

We thus read off the ingredients of  $\mathcal{A} = |\sigma_1\rangle_1 A^{\sigma_1}$  and  $\mathcal{B} = |\sigma_2\rangle_2 B^{\sigma_2}$  as follows:

$$\mathcal{A} = |0\rangle_1 \underbrace{\begin{pmatrix} 1 & 0 \end{pmatrix}}_{A^{\sigma_1=0}} + |1\rangle_1 \underbrace{\begin{pmatrix} 0 & 1 \end{pmatrix}}_{A^{\sigma_1=1}}, \quad \mathcal{B} = |0\rangle_2 \underbrace{\begin{pmatrix} 1 \\ 0 \end{pmatrix}}_{B^{\sigma_2=0}} + |1\rangle_2 \underbrace{\begin{pmatrix} 0 \\ 1 \end{pmatrix}}_{B^{\sigma_2=1}}.$$

[ii] *Generalize to an arbitrary  $N$ .* Since  $|\text{GHZN}\rangle$  contains terms involving only products of  $|0\rangle_\ell$ s or products of  $|1\rangle_\ell$ s,

$$|\text{GHZN}\rangle = \frac{1}{\sqrt{2}}(|0, \dots, 0\rangle + |1, \dots, 1\rangle) = \frac{1}{\sqrt{2}}(|0\rangle_1 \dots |1\rangle_N) \mathcal{M}_2 \dots \mathcal{M}_{N-1} \begin{pmatrix} |0\rangle_N \\ |1\rangle_N \end{pmatrix},$$

we read off the ingredients of  $\mathcal{M}_\ell = |\sigma_\ell\rangle_\ell M^{\sigma_\ell}$  as follows:

$$\mathcal{M}_\ell = \begin{pmatrix} |0\rangle_\ell & 0 \\ 0 & |1\rangle_\ell \end{pmatrix}, \quad (M_\ell)^{\sigma_\ell=0} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad (M_\ell)^{\sigma_\ell=1} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}.$$

[iii] *Canonical MPS.* The MPS representation of  $|\text{GHZN}\rangle$  reads:

$$\frac{1}{\sqrt{2}} \left( \begin{array}{c} \text{---} M_1 \text{---} M_2 \text{---} \dots \text{---} M_N \text{---} \\ \text{---} \sigma_1 \text{---} \sigma_2 \text{---} \dots \text{---} \sigma_N \text{---} \end{array} \right)$$

This MPS is left-canonical if the prefactor  $\frac{1}{\sqrt{2}}$  is absorbed into  $\mathcal{M}_N$ , or right-canonical if the prefactor is absorbed in to  $\mathcal{M}_1$ :

$$\text{left-canonical:} \quad \alpha_{\ell-1} \begin{array}{c} \text{---} M_\ell \text{---} \\ \text{---} \sigma_\ell \text{---} \\ \text{---} M_\ell^\dagger \text{---} \end{array} \alpha'_\ell = \begin{pmatrix} \alpha_\ell \\ \alpha'_\ell \end{pmatrix}, \quad \alpha_{N-1} \begin{array}{c} \text{---} M_N/\sqrt{2} \text{---} \\ \text{---} \sigma_N \text{---} \\ \text{---} M_N^\dagger/\sqrt{2} \text{---} \end{array} = 1. \quad (1)$$

$$\text{right-canonical:} \quad \alpha_{\ell-1} \begin{array}{c} \text{---} M_\ell \text{---} \\ \text{---} \sigma_\ell \text{---} \\ \text{---} M_\ell^\dagger \text{---} \end{array} \alpha_\ell = \begin{pmatrix} \alpha_{\ell-1} \\ \alpha'_\ell \end{pmatrix}, \quad \begin{array}{c} \text{---} M_1/\sqrt{2} \text{---} \\ \text{---} \sigma_1 \text{---} \\ \text{---} M_1^\dagger/\sqrt{2} \text{---} \end{array} \alpha_1 = 1. \quad (2)$$

(iv) *SVD and MPS.* We verify the observation in [iii] as follows.

```

1 using LinearAlgebra
2 using Printf
3
4 include("Tensor.jl")
5
6 N = 10
7 GHZ_N = zeros(2^10, 1)
8 GHZ_N[1] = 1/sqrt(2); # |0,...,0>/sqrt(2)
9 GHZ_N[end] = 1/sqrt(2); # |1,...,1>/sqrt(2)
10
11 M = Array{Any}(undef, 1, N);
12 T = reshape(GHZ_N*sqrt(2), (1, 2, length(GHZ_N)/2))
13 for itN = (1:N-1)
14     global T
15     U, S, Vd = svdTr(T, 3, [1, 2], Inf, 0)
16     M[itN] = U
17     T = contract(diagm(S), 2, 2, Vd, 2, 1)
18     T = reshape(T, (size(T, 1), 2, size(T, 2)/2))
19 end
20 M[end] = T
```

```

21
22 # check left canonical
23 M_N = M[N]/sqrt(2)
24 for itN in (1:N)
25     if itN < N
26         MM = contract(M[itN],3,[1,2],conj(M[itN]),3,[1,2])
27     else
28         MM = contract(M_N,3,[1,2],conj(M_N),3,[1,2])
29     end
30     Id = I(size(MM,1))
31     err = norm(MM-Id)
32     @printf("norm of difference between MM* and the expected identity matrix at site
           %d: %.4e\n",itN,err)
33 end
34
35 # check right canonical
36 M_1 = M[1]/sqrt(2)
37 for itN in (1:N)
38     if itN > 1
39         MM = contract(M[itN],3,[2,3],conj(M[itN]),3,[2,3])
40     else
41         MM = contract(M_1,3,[2,3],conj(M_1),3,[2,3])
42     end
43     Id = I(size(MM,1))
44     err = norm(MM-Id)
45     @printf("norm of difference between MM* and the expected identity matrix at site
           %d: %.4e\n",itN,err)
46 end
47
48 # Nkeep = 2
49 Nkeep = 2
50 dw_set = zeros(N-1,1)
51 T = reshape(GHZ_N*sqrt(2), (1,2,length(GHZ_N)/2))
52 for itN = (1:N-1)
53     global T
54     U,S,Vd,dw = svdTr(T,3,[1,2],Nkeep,0)
55     M[itN] = U
56     dw_set[itN] = dw
57     T = contract(diagm(S),2,2,Vd,2,1)
58     T = reshape(T, (size(T,1),2,size(T,2)/2))
59     @printf("discarded weight of the SVD on site %d: %f\n",itN,dw_set[itN])
60 end
61
62 # Nkeep = 1
63 Nkeep = 1
64 dw_set = zeros(N-1,1)
65 T = reshape(GHZ_N*sqrt(2), (1,2,length(GHZ_N)/2))
66 for itN = (1:N-1)
67     global T
68     U,S,Vd,dw = svdTr(T,3,[1,2],Nkeep,0)
69     M[itN] = U
70     dw_set[itN] = dw
71     T = contract(diagm(S),2,2,Vd,2,1)
72     T = reshape(T, (size(T,1),2,size(T,2)/2))
73     # note that the discarded weight is nonzero for itN = 1
74     @printf("discarded weight of the SVD on site %d: %f\n",itN,dw_set[itN])
75 end

```

For  $N_{\text{keep}}=\infty$ , the resulting MPS is left-canonical (or right-canonical) if the prefactor  $\frac{1}{\sqrt{2}}$  is absorbed into  $\mathcal{M}_1$  (or  $\mathcal{M}_N$ ) as found in (iii). For  $N_{\text{keep}}=2$ , the discarded weights are all 0, because the bond dimensions of  $\alpha_\ell$  for  $\mathcal{M}_\ell$  is  $D = 2$ . Since all weights are kept, the resulting MPS tensor agrees with the one found in (iii). However, for  $N_{\text{keep}}=1$ , some discarded weight(s) are nonzero.

## Solution T03.2: Matrix product operators [6]

### (a) Spin Systems

[(i)] *Spin- $\frac{1}{2}$  Ising model.* [1] The MPO ingredients  $W_1$  or  $W_{\mathcal{L}}$  are the last row vector or the first column vector of  $W_{\ell}$ , respectively:

$$W_1 = \begin{pmatrix} 0 & JS_1^z & \mathbb{1}_1 \end{pmatrix}, \quad W_{\mathcal{L}} = \begin{pmatrix} \mathbb{1}_{\mathcal{L}} \\ S_{\mathcal{L}}^z \\ 0 \end{pmatrix}.$$

To verify that this works, multiply out the MPO matrices for a short chain, e.g.  $\mathcal{L} = 3$ :

$$\begin{aligned} W_1 W_2 W_3 &= \begin{pmatrix} 0 & JS_1^z & \mathbb{1}_1 \end{pmatrix} \begin{pmatrix} \mathbb{1}_2 & 0 & 0 \\ S_2^z & 0 & 0 \\ 0 & JS_2^z & \mathbb{1}_2 \end{pmatrix} \begin{pmatrix} \mathbb{1}_3 \\ S_3^z \\ 0 \end{pmatrix} = \begin{pmatrix} 0 & JS_1^z & \mathbb{1}_1 \end{pmatrix} \begin{pmatrix} \mathbb{1}_2 \mathbb{1}_3 \\ S_2^z \mathbb{1}_3 \\ JS_2^z S_3^z \end{pmatrix} \\ &= J(S_1^z S_2^z \mathbb{1}_3 + \mathbb{1}_1 S_2^z S_3^z). \end{aligned}$$

(2) We now explicitly construct the MPO ingredient  $W_{\ell}$ , and multiply out the MPO to verify that it reproduces the Hamiltonian  $H_{\text{Ising}}$ :

```

1 using LinearAlgebra
2 using Printf
3
4 include("Tensor.jl")
5
6 J = 1
7 L = 4
8 Sz = [1 0; 0 -1]/2
9 W = Array{Any}(undef,1,L); # MPO W
10 # first site
11 W[1] = zeros(1,2,3,2); # leg ordering: left bottom right top
12 W[1][1, :, 2, :] = J*Sz; # J*S_1^z
13 W[1][1, :, 3, :] = I(2); # I
14 # sites between first & last sites
15 for itW in (2:L-1)
16     W[itW] = zeros(3,2,3,2); # leg ordering: left bottom right top
17     W[itW][1, :, 1, :] = I(2); # I
18     W[itW][2, :, 1, :] = Sz; # S_itW^z
19     W[itW][3, :, 2, :] = J*Sz; # J*S_itW^z
20     W[itW][3, :, 3, :] = I(2); # I
21 end
22 # last site
23 W[L] = zeros(3,2,1,2); # left ordering: left bottom right top
24 W[L][1, :, 1, :] = I(2); # I
25 W[L][2, :, 1, :] = Sz; # S_L^z
26 ##
27 # The MPOs are multiplied together & compared with the full Hamiltonian for
28 # $\mathcal{L}=4$.
29
30 H_MPO = reshape([1],(1,1,1,1)); # Full Hamiltonian constructed from MPO W
31 for itW in (1:L)
32     global H_MPO
33     H_MPO = contract(H_MPO,4,3,W[itW],4,1)
34     H_MPO = permutedims(H_MPO,(1,2,4,5,3,6))
35     # reshape H_MPO to be a rank-4 tensor
36     H_MPO = reshape(H_MPO,(size(H_MPO,1),
37                                     size(H_MPO,2)*size(H_MPO,3),
38                                     size(H_MPO,4),
39                                     size(H_MPO,5)*size(H_MPO,6)))
40 end
41 H_MPO = reshape(H_MPO,(size(H_MPO,2),size(H_MPO,4)))
42
43 # H_dir: Full Hamiltonian constructed directly
44 Sz1 = kron(Sz,kron(I(2),kron(I(2),I(2))))
45 Sz2 = kron(I(2),kron(Sz,kron(I(2),I(2))))
46 Sz3 = kron(I(2),kron(I(2),kron(Sz,I(2))))
47 Sz4 = kron(I(2),kron(I(2),kron(I(2),Sz)))
48 H_dir = J*(Sz1*Sz2+Sz2*Sz3+Sz3*Sz4)
49 # comparing H_MPO & H_dir
50 diff = norm(H_dir-H_MPO)

```

51 @printf("Norm of difference between H\_MPO & H\_dir: %e %%",diff)

[ii] *Spin- $\frac{1}{2}$  XY model.* The Hamiltonian for the XY model can be phrased as an MPO with bond dimension  $D_W = 4$ , using the ingredients

$$W_1 = \begin{pmatrix} 0 & JS_1^x & JS_1^y & \mathbb{1}_1 \end{pmatrix}, \quad W_\ell = \begin{pmatrix} \mathbb{1}_\ell & 0 & 0 & 0 \\ S_\ell^x & 0 & 0 & 0 \\ S_\ell^y & 0 & 0 & 0 \\ 0 & JS_\ell^x & JS_\ell^y & \mathbb{1}_\ell \end{pmatrix}, \quad W_{\mathcal{L}} = \begin{pmatrix} \mathbb{1}_{\mathcal{L}} \\ S_{\mathcal{L}}^x \\ S_{\mathcal{L}}^y \\ 0 \end{pmatrix}.$$

To verify that this works, multiply out the MPO matrices for a short chain, e.g.  $\mathcal{L} = 3$ :

$$\begin{aligned} W_1 W_2 W_3 &= \begin{pmatrix} 0 & JS_1^x & JS_1^y & \mathbb{1}_1 \end{pmatrix} \begin{pmatrix} \mathbb{1}_2 & 0 & 0 & 0 \\ S_2^x & 0 & 0 & 0 \\ S_2^y & 0 & 0 & 0 \\ 0 & JS_2^x & JS_2^y & \mathbb{1}_2 \end{pmatrix} \begin{pmatrix} \mathbb{1}_3 \\ S_3^x \\ S_3^y \\ 0 \end{pmatrix} \\ &= \begin{pmatrix} 0 & JS_1^x & JS_1^y & \mathbb{1}_1 \end{pmatrix} \begin{pmatrix} \mathbb{1}_2 \mathbb{1}_3 \\ S_2^x \mathbb{1}_3 \\ S_2^y \mathbb{1}_3 \\ J(S_2^x S_3^x + S_2^y S_3^y) \end{pmatrix} \\ &= J(S_1^x S_2^x \mathbb{1}_3 + S_1^y S_2^y \mathbb{1}_3 + \mathbb{1}_1 S_2^x S_3^x + \mathbb{1}_1 S_2^y S_3^y). \end{aligned}$$

The term  $h_\ell S_\ell^z$  can be included in  $W_\ell$  as

$$W_1 = \begin{pmatrix} h_1 S_1^z & JS_1^x & JS_1^y & \mathbb{1}_1 \end{pmatrix}, \quad W_\ell = \begin{pmatrix} \mathbb{1}_\ell & 0 & 0 & 0 \\ S_\ell^x & 0 & 0 & 0 \\ S_\ell^y & 0 & 0 & 0 \\ h_\ell S_\ell^z & JS_\ell^x & JS_\ell^y & \mathbb{1}_\ell \end{pmatrix}, \quad W_{\mathcal{L}} = \begin{pmatrix} \mathbb{1}_{\mathcal{L}} \\ S_{\mathcal{L}}^x \\ S_{\mathcal{L}}^y \\ h_{\mathcal{L}} S_{\mathcal{L}}^z \end{pmatrix}.$$

To verify that this works, multiply out the MPO matrices for a short chain, e.g.  $\mathcal{L} = 3$ :

$$\begin{aligned} W_1 W_2 W_3 &= \begin{pmatrix} h_1 S_1^z & JS_1^x & JS_1^y & \mathbb{1}_1 \end{pmatrix} \begin{pmatrix} \mathbb{1}_2 & 0 & 0 & 0 \\ S_2^x & 0 & 0 & 0 \\ S_2^y & 0 & 0 & 0 \\ h_2 S_2^z & JS_2^x & JS_2^y & \mathbb{1}_2 \end{pmatrix} \begin{pmatrix} \mathbb{1}_3 \\ S_3^x \\ S_3^y \\ h_3 S_3^z \end{pmatrix} \\ &= \begin{pmatrix} h_1 S_1^z & JS_1^x & JS_1^y & \mathbb{1}_1 \end{pmatrix} \begin{pmatrix} \mathbb{1}_2 \mathbb{1}_3 \\ S_2^x \mathbb{1}_3 \\ S_2^y \mathbb{1}_3 \\ h_2 S_2^z \mathbb{1}_3 + h_3 \mathbb{1}_2 S_3^z + J(S_2^x S_3^x + S_2^y S_3^y) \end{pmatrix} \\ &= h_1 S_1^z \mathbb{1}_2 \mathbb{1}_3 + h_3 \mathbb{1}_1 S_2^z \mathbb{1}_3 + h_3 \mathbb{1}_1 \mathbb{1}_2 S_3^z + J(S_1^x S_2^x \mathbb{1}_3 + S_1^y S_2^y \mathbb{1}_3 + \mathbb{1}_1 S_2^x S_3^x + \mathbb{1}_1 S_2^y S_3^y). \end{aligned}$$

[(iii)] *Exponential long-range interactions.* [1] These can be encoded in  $W_\ell$  with  $D_W = 3$  as

$$W_1 = \begin{pmatrix} 0 & e^{-\lambda} S_1^z & \mathbb{1}_1 \end{pmatrix}, \quad W_\ell = \begin{pmatrix} \mathbb{1}_\ell & 0 & 0 \\ S_\ell^z & e^{-\lambda} \mathbb{1}_\ell & 0 \\ 0 & e^{-\lambda} S_\ell^z & \mathbb{1}_\ell \end{pmatrix}, \quad W_{\mathcal{L}} = \begin{pmatrix} \mathbb{1}_{\mathcal{L}} \\ S_{\mathcal{L}}^z \\ 0 \end{pmatrix}$$

To verify that this works, multiply out the MPO matrices for a short chain, e.g.  $\mathcal{L} = 3$ :

$$W_1 W_2 W_3 = \begin{pmatrix} \mathbb{1}_2 & 0 & 0 \\ S_2^z & e^{-\lambda} \mathbb{1}_2 & 0 \\ 0 & e^{-\lambda} S_2^z & \mathbb{1}_2 \end{pmatrix} \begin{pmatrix} \mathbb{1}_3 \\ S_3^z \\ 0 \end{pmatrix} = \begin{pmatrix} 0 & e^{-\lambda} S_1^z & \mathbb{1}_1 \end{pmatrix} \begin{pmatrix} \mathbb{1}_2 \mathbb{1}_3 \\ S_2^z \mathbb{1}_3 + e^{-\lambda} \mathbb{1}_2 S_3^z \\ e^{-\lambda} S_2^z S_3^z \end{pmatrix}$$

$$= e^{-\lambda} (S_1^z S_2^z \mathbb{1}_3 + \mathbb{1}_1 S_2^z S_3^z) + e^{-2\lambda} S_1^z \mathbb{1}_2 S_3^z.$$

(2) We implement the Hamiltonian  $-H_{\lambda=1}$  and show that the state  $|\downarrow \dots \downarrow\rangle$  is an eigenstate:

```

1 using LinearAlgebra
2 using Printf
3
4 include("Tensor.jl")
5
6 L = 6
7 lambda = 1;
8 Sz = [1 0; 0 -1]/2
9 W = Array{Any}(undef, 1, L); # MPO W
10 # first site
11 W[1] = zeros(3, 2, 3, 2); # leg ordering: left bottom right top
12 W[1][1, :, 2, :] = -exp(-lambda)*Sz; # J*S_1^z
13 W[1][1, :, 3, :] = I(2); # I
14 # sites between first & last sites
15 for itW in (2:L-1)
16     W[itW] = zeros(3, 2, 3, 2); # leg ordering: left bottom right top
17     W[itW][1, :, 1, :] = I(2); # I
18     W[itW][2, :, 1, :] = Sz; # S_itW^z
19     W[itW][2, :, 2, :] = exp(-lambda)*I(2); # e^(lambda)*I
20     W[itW][3, :, 2, :] = -exp(-lambda)*Sz; # J*S_itW^z
21     W[itW][3, :, 3, :] = I(2); # I
22 end
23 # last site
24 W[L] = zeros(3, 2, 1, 2); # left ordering: left bottom right top
25 W[L][1, :, 1, :] = I(2); # I
26 W[L][2, :, 1, :] = Sz; # S_L^z
27 ##
28 # The MPOs are multiplied together & compared with the full Hamiltonian for
29 # $\mathcal{L}=4$.
30
31 Psi = zeros(2^L, 1);
32 Psi[end] = 1; # |Psi> = |down_arrow ... down_arrow>
33
34 H_MPO = reshape([1], (1, 1, 1, 1)); # Full Hamiltonian constructed from MPO W
35 for itW in (1:L)
36     global H_MPO
37     H_MPO = contract(H_MPO, 4, 3, W[itW], 4, 1)
38     H_MPO = permutedims(H_MPO, (1, 2, 4, 5, 3, 6))
39     # reshape H_MPO to be a rank-4 tensor
40     H_MPO = reshape(H_MPO, (size(H_MPO, 1),
41                             size(H_MPO, 2)*size(H_MPO, 3),
42                             size(H_MPO, 4),
43                             size(H_MPO, 5)*size(H_MPO, 6)))
44 end
45 H_MPO = reshape(H_MPO, (size(H_MPO, 2), size(H_MPO, 4)))
46
47 HPsi = H_MPO*Psi; # H|Psi>
48 HPsi = HPsi/norm(HPsi); # normalize H|Psi>
49 P_Psi = Psi'*Psi; # Projection on the Psi
50 diff = norm(P_Psi*HPsi - HPsi); # if P(H|Psi>) = H|Psi>, then H|Psi> = |Psi>
51 @printf("Norm of difference between PH|Psi> and H|Psi>: %e %%", diff)

```

## (b) Fermionic systems

[i] *Spinless tight-binding free fermions*. To keep track of fermion signs, we introduce  $z$  factors:

$$\hat{c}_\ell^\dagger \hat{c}_{\ell+1} = (c_\ell^\dagger z_{\ell+1} z_{\ell+2} \dots z_{\mathcal{L}}) (c_{\ell+1} z_{\ell+2} \dots \times z_{\mathcal{L}}) = c_\ell^\dagger z_{\ell+1} c_{\ell+1} = c_\ell^\dagger c_{\ell+1}, \quad (3)$$

$$\hat{c}_{\ell+1}^\dagger \hat{c}_\ell = (c_{\ell+1}^\dagger z_{\ell+2} \dots z_{\mathcal{L}}) (c_\ell z_{\ell+1} z_{\ell+2} \dots \times z_{\mathcal{L}}) = c_{\ell+1}^\dagger z_{\ell+1} c_\ell = c_{\ell+1}^\dagger c_\ell. \quad (4)$$

For the last steps on the right we exploited the fact that  $c_\ell^\dagger z_{\ell+1} = c_\ell^\dagger$  and  $z_{\ell+1} c_\ell = c_\ell$ , since these operators are nonzero only when acting on  $|0\rangle_\ell$  or  $|1\rangle_\ell$ , respectively. Hence, all  $z$  factors drop out, and we choose

$$W_1 = \begin{pmatrix} \mathbb{1}_\ell & 0 & 0 & 0 \\ 0 & tc_1^\dagger & tc_1 & \mathbb{1}_1 \end{pmatrix}, \quad W_\ell = \begin{pmatrix} \mathbb{1}_\ell & 0 & 0 & 0 \\ c_\ell & 0 & 0 & 0 \\ c_\ell^\dagger & 0 & 0 & 0 \\ 0 & tc_\ell^\dagger & tc_\ell & \mathbb{1}_\ell \end{pmatrix}, \quad W_{\mathcal{L}} = \begin{pmatrix} \mathbb{1}_{\mathcal{L}} \\ c_{\mathcal{L}} \\ c_{\mathcal{L}}^\dagger \\ 0 \end{pmatrix}.$$

[ii] *Jordan–Wigner transformation.* Under the Jordan-Wigner transformation,  $\hat{c}_\ell^\dagger \hat{c}_{\ell+1}$  and  $\hat{c}_{\ell+1}^\dagger \hat{c}_\ell$  become as follows:

$$\hat{c}_\ell^\dagger \hat{c}_{\ell+1} = (\sigma_1^z \dots \sigma_{\ell-1}^z \sigma_\ell^+) (\sigma_1^z \dots \sigma_{\ell-1}^z \sigma_\ell^- \sigma_{\ell+1}^-) = \sigma_\ell^+ \sigma_\ell^- \sigma_{\ell+1}^- = -\sigma_\ell^+ \sigma_{\ell+1}^-, \quad (5)$$

$$\hat{c}_{\ell+1}^\dagger \hat{c}_\ell = (\sigma_1^z \dots \sigma_{\ell-1}^z \sigma_\ell^+ \sigma_{\ell+1}^-) (\sigma_1^z \dots \sigma_{\ell-1}^z \sigma_\ell^-) = \sigma_{\ell+1}^+ \sigma_\ell^- \sigma_\ell^- = -\sigma_{\ell+1}^+ \sigma_\ell^-. \quad (6)$$

For the last steps on the right we exploited the fact that  $\sigma_\ell^+ \sigma_\ell^- = -\sigma_\ell^+$  and  $\sigma_\ell^- \sigma_\ell^+ = -\sigma_\ell^-$  since these operators are nonzero only when acting on  $|\downarrow\rangle_\ell$  or  $|\uparrow\rangle_\ell$ , respectively. Hence, all  $\sigma_\ell^\pm$  drop out, and we choose

$$W_1 = \begin{pmatrix} \mathbb{1}_\ell & 0 & 0 & 0 \\ 0 & -t\sigma_1^+ & -t\sigma_1^- & \mathbb{1}_1 \end{pmatrix}, \quad W_\ell = \begin{pmatrix} \mathbb{1}_\ell & 0 & 0 & 0 \\ \sigma_\ell^- & 0 & 0 & 0 \\ \sigma_\ell^+ & 0 & 0 & 0 \\ 0 & -t\sigma_\ell^+ & -t\sigma_\ell^- & \mathbb{1}_\ell \end{pmatrix}, \quad W_{\mathcal{L}} = \begin{pmatrix} \mathbb{1}_{\mathcal{L}} \\ \sigma_{\mathcal{L}}^- \\ \sigma_{\mathcal{L}}^+ \\ 0 \end{pmatrix}.$$

The  $W_\ell$  matrices from [i] and [ii] are identical, up to  $t \leftrightarrow -t$ . This reflects the fact that for spinless fermions,  $H_{\text{ff}} = t \sum_{\langle \ell \bar{\ell} \rangle} (c_\ell^\dagger c_{\bar{\ell}} + c_{\bar{\ell}}^\dagger c_\ell)$  is equivalent to the spinflip Hamiltonian  $-t \sum_{\langle \ell \bar{\ell} \rangle} (\sigma_\ell^+ \sigma_{\bar{\ell}}^- + \sigma_\ell^- \sigma_{\bar{\ell}}^+)$ .

[iii] *Fourier transform.* The operator  $c_k^\dagger$  can be expressed as the MPO of  $D_W = 2$  as follows.

$$W_1 = \begin{pmatrix} e^{ik} c_1^\dagger & \mathbb{1}_1 \end{pmatrix}, \quad W_\ell = \begin{pmatrix} z_\ell & 0 \\ e^{ik\ell} c_\ell^\dagger & \mathbb{1}_\ell \end{pmatrix}, \quad W_{\mathcal{L}} = \begin{pmatrix} z_{\mathcal{L}} \\ e^{ik\mathcal{L}} c_{\mathcal{L}}^\dagger \end{pmatrix}.$$

To verify that this works, multiply out the MPO matrices for a short chain, e.g.,  $\mathcal{L} = 3$ :

$$\begin{aligned} W_1 W_2 W_3 &= \begin{pmatrix} e^{ik} c_1^\dagger & \mathbb{1}_1 \end{pmatrix} \begin{pmatrix} z_2 & 0 \\ e^{2ik} c_2^\dagger & \mathbb{1}_2 \end{pmatrix} \begin{pmatrix} z_3 \\ e^{3ik} c_3^\dagger \end{pmatrix} = \begin{pmatrix} e^{ik} c_1^\dagger & \mathbb{1}_1 \end{pmatrix} \begin{pmatrix} z_2 z_3 \\ e^{2ik} c_2^\dagger z_3 + e^{3ik} \mathbb{1}_2 c_3^\dagger \end{pmatrix} \\ &= e^{ik} c_1^\dagger z_2 z_3 + e^{2ik} \mathbb{1}_1 c_2^\dagger z_3 + e^{3ik} \mathbb{1}_1 \mathbb{1}_2 c_3^\dagger = \sum_\ell e^{ik\ell} \hat{c}_\ell^\dagger. \end{aligned}$$

### Solution T03.3: Iterative diagonalization and MPOs [5]

#### (a) Spin systems

(i) *Verify your MPO implementation.* (1) We compute the ground state  $|\Psi_{\text{MPS}}\rangle$  and its energy  $E_{\text{MPS}}$ . (2) We construct the MPO for the XY Hamiltonian. (3) We verify that the energy  $E_{\text{MPO}}$  agrees with  $E_{\text{MPS}}$  within machine precision.

```

1  using LinearAlgebra
2  using Printf
3  using JLD2
4
5  include("Tensor.jl");
6
7  J = 1;
8  L = 50; # maximum chain length
9  Nkeep = 300; # maximal number of states to keep
10 S, Id = getLocalSpace("Spin", 1/2)
11
12 @printf("Iterative Diagonalization\n")
13
14 H0 = Id*0; # Hamiltonian for only the 1st site
15 A0 = getIdentity(1,2,Id,2); # 1st leg is dummy leg (vacuum)
16
17 # MPS of the GS
18 MPS = Array{Any}(undef, 1, L);
19
20 # initialization
21 Hnow = H0
22 D, V = eigen((Hnow+Hnow')/2)
23 MPS[1] = contract(A0, 3, 3, V, 2, 1)
24 Hprev = diagm(D)
25
26 for itL in (2:L)
27
28     global A, Hprev, Eg_Iter;
29
30     # step [i-ii]
31     # spin operator at the current site; to be used for generating
32     # the coupling term at the next iteration
33     Sprex = updateLeft([], [], MPS[itL-1], S, 3, MPS[itL-1])
34
35     # step [iii]
36     # # add new site
37     Anow = getIdentity(Hprev, 2, Id, 2)
38     Hnow = updateLeft(Hprev, 2, Anow, [], [], Anow)
39     # update the Hamiltonian up to the last sites
40     # to the enlarged Hilbert space
41
42     # step [iv]
43     # # spin-spin interaction
44     Sprex_x = (Sprex[:, 1, :] + Sprex[:, 2, :])/sqrt(2); Rx = size(Sprex_x);
45     Sprex_y = (Sprex[:, 1, :] - Sprex[:, 2, :])/sqrt(2)/1im; Ry = size(Sprex_y);
46     if length(Rx) == 2; Sprex_x = reshape(Sprex_x, (Rx[1], 1, Rx[2])); end;
47     if length(Ry) == 2; Sprex_y = reshape(Sprex_y, (Ry[1], 1, Ry[2])); end;
48     Sx = reshape((S[:, 1, :] + S[:, 2, :])/sqrt(2), (2, 1, 2));
49     Sy = reshape((S[:, 1, :] - S[:, 2, :])/sqrt(2)/1im, (2, 1, 2));
50     Hxy = J * updateLeft(Sprex_x, 3, Anow, Sx, 3, Anow) + J * updateLeft(Sprex_y, 3, Anow,
51         Sy, 3, Anow)
52
53     # step [v]
54     Hnow = Hnow+Hxy
55
56     # diagonalize the current Hamiltonian
57     D, V = eigen((Hnow+Hnow')/2)
58     # sort eigenvalues & eigenvectors in the order of increasing
59     # eigenvalues
60     ids = sortperm(D)
61     D = D[ids]
62     V = V[:, ids]
63
64     if itL == L; Eg_Iter = minimum(D); end
65
66     # truncation threshold for energy
67     Etr = D[min(length(D), Nkeep)]
68     oks = (D .< Etr)
69     # true: to keep; false: not to keep
70     # keep all degenerate states up to tolerance
71
72     if itL < L
73         MPS[itL] = contract(Anow, 3, 3, V[:, oks], 2, 1)
74     else
75         MPS[itL] = contract(Anow, 3, 3, reshape(V[:, 1], (size(V[:, 1])[1], 1)), 2, 1) #
76             select GS at the last step

```



```

75     end
76     Hprev = diagm(D[oks])
77
78 end
79
80
81 @printf("MPS/MPO Contraction\n")
82
83 Sx = reshape((S[:,1,:]+S[:,2,:])/sqrt(2),(2,1,2));
84 Sy = reshape((S[:,1,:]-S[:,2,:])/sqrt(2)/1im,(2,1,2));
85
86 W = Array{Any}(undef,1,L); # MPO W
87 # first site
88 W[1] = zeros(Complex{Float64},1,2,4,2); # ordering: left bottom right top
89 W[1][1, :, 2, :] = J*Sx; # J*S_1^x
90 W[1][1, :, 3, :] = J*Sy; # J*S_1^y
91 W[1][1, :, 4, :] = I(2); # I
92 # sites between first & last sites
93 for itW in (2:L-1)
94     W[itW] = zeros(Complex{Float64},4,2,4,2); # ordering: left bottom right top
95     W[itW][1, :, 1, :] = I(2); # I
96     W[itW][2, :, 1, :] = Sx; # S_itW^x
97     W[itW][3, :, 1, :] = Sy; # S_itW^y
98     W[itW][4, :, 2, :] = J*Sx; # J*S_itW^x
99     W[itW][4, :, 3, :] = J*Sy; # J*S_itW^y
100    W[itW][4, :, 4, :] = I(2); # I
101 end
102 # last site
103 W[L] = zeros(Complex{Float64},4,2,1,2); # ordering: left bottom right top
104 W[L][1, :, 1, :] = I(2); # I
105 W[L][2, :, 1, :] = Sx; # S_L^x
106 W[L][3, :, 1, :] = Sy; # S_L^y
107
108
109 Eg_MPO = reshape([1],(1,1,1));
110 for itL in (1:L)
111     global Eg_MPO
112     Eg_MPO = updateLeft(Eg_MPO,3,MPS[itL],W[itL],4,MPS[itL]);
113 end
114
115 @save "GSEnergies.jld2" Eg_Iter Eg_MPO
116
117 diff = Eg_Iter - Eg_MPO[1];
118 @printf("Difference between Eg_Iter and Eg_MPO: %.4f\n", diff)

```

## (b) Fermionic systems

(i) *Iterative diagonalization.* Under the Jordan-Wigner transformation, the Hamiltonian  $H_{\text{ff}}$  is mapped to  $H_{\text{ff}} = -t \sum_{\ell} (\sigma_{\ell}^{+} \sigma_{\ell+1}^{-} + \text{h.c.})$ . The diagonalization of this Hamiltonian is described below. The ground state energy of  $H_{\text{ff}}$  is found to agree with that of  $H_{\text{XY}}$  from (a).

```

1 using LinearAlgebra
2 using Printf
3 using JLD2
4
5 include("Tensor.jl");
6
7 @load "GSEnergies.jld2"
8
9 t = 0.5;
10 L = 50; # maximum chain length()
11 Nkeep = 300; # maximal number of states to keep
12 S, Id = getLocalSpace("Spin",1/2)
13
14 @printf("Iterative Diagonalization\n")
15
16 H0 = Id*0; # Hamiltonian for only the 1st site
17 A0 = getIdentity(1,2,Id,2); # 1st leg is dummy leg (vacuum)
18
19 # MPS of the GS
20 MPS = Array{Any}(undef,1,L);
21
22 # initialization
23 Hnow = H0

```

```

24 D,V = eigen((Hnow+Hnow')/2)
25 MPS[1] = contract(A0,3,3,V,2,1)
26 Hprev = diagm(D)
27
28 # sigma_+ sigma_z
29 SpSz = contract(reshape(sqrt(2)*S[:,1,:],(2,1,2)),3,3,
30 reshape(2*S[:,3,:],(2,2)),2,1);
31 # sigma_z sigma_-
32 SzSm = contract(reshape(2*S[:,3,:],(2,2)),2,2,
33 reshape(sqrt(2)*S[:,2,:],(2,1,2)),3,1);
34
35 for itL in (2:L)
36
37     global A, Hprev, SpSz, SzSm, Eg_IterF;
38
39     # step [i-ii]
40     # spin operator at the current site; to be used for generating
41     # the coupling term at the next iteration
42     SpSz_prev = updateLeft([],[],MPS[itL-1],SpSz,3,MPS[itL-1]);
43     SzSm_prev = updateLeft([],[],MPS[itL-1],SzSm,3,MPS[itL-1]);
44
45     # step [iii]
46     # # add new site
47     Anow = getIdentity(Hprev,2,Id,2)
48     Hnow = updateLeft(Hprev,2,Anow,[],[],Anow)
49     # update the Hamiltonian up to the last sites
50     # to the enlarged Hilbert space
51
52     # step [iv]
53     # # spin-spin interaction
54     Hxy = t * updateLeft(SpSz_prev,3,Anow,reshape(sqrt(2)*S[:,2,:],(2,1,2)),3,Anow)
55         + t * updateLeft(SzSm_prev,3,Anow,reshape(sqrt(2)*S[:,1,:],(2,1,2)),3,Anow)
56         ;
57
58     # step [v]
59     Hnow = Hnow+Hxy
60
61     # diagonalize the current Hamiltonian
62     D,V = eigen((Hnow+Hnow')/2)
63     # sort eigenvalues & eigenvectors in the order of increasing
64     # eigenvalues
65     ids = sortperm(D)
66     D = D[ids]
67     V = V[:,ids]
68
69     if itL == L; Eg_IterF = minimum(D); end
70
71     # truncation threshold for energy
72     Etr = D[min(length(D),Nkeep)]
73     oks = (D .< Etr)
74     # true: to keep; false: not to keep
75     # keep all degenerate states up to tolerance
76
77     if itL < L
78         MPS[itL] = contract(Anow,3,3,V[:,oks],2,1)
79     else
80         MPS[itL] = contract(Anow,3,3,reshape(V[:,1],(size(V[:,1])[1],1)),2,1) #
81         select GS at the last step
82     end
83     Hprev = diagm(D[oks])
84
85 end
86
87 @save "MPS.jld2" MPS
88
89 @printf("Ground state energy of Fermionic chain: %.4f\n", Eg_IterF)
90
91 diff = Eg_Iter - Eg_IterF[1];
92 @printf("Difference between Eg_Iter and Eg_IterF: %.4f\n", diff)

```

(ii) *MPO for Hamiltonian.* The construction of the MPO for  $H_{\text{ff}}$  is described below. The energy  $E_{\text{MPS}}$  from (i) is reproduced.

```

1 using LinearAlgebra
2 using Printf

```

```

3 using JLD2
4
5 include("Tensor.jl");
6
7 @load "GSEnergies.jld2"
8 @load "MPS.jld2"
9
10 t = 0.5;
11 L = 50; # maximum chain length
12 S, Id = getLocalSpace("Spin", 1/2)
13
14 W = Array{Any}(undef, 1, L); # MPO W
15 # first site
16 W[1] = zeros(Complex{Float64}, 1, 2, 4, 2); # ordering: left bottom right top
17 W[1][1, :, 2, :] = -t*sqrt(2)*S[:, 1, :]; # t*S_1^x
18 W[1][1, :, 3, :] = -t*sqrt(2)*S[:, 2, :]; # t*S_1^y
19 W[1][1, :, 4, :] = Id; # I
20 # sites between first & last sites
21 for itW in (2:L-1)
22     W[itW] = zeros(Complex{Float64}, 4, 2, 4, 2); # ordering: left bottom right top
23     W[itW][1, :, 1, :] = Id; # I
24     W[itW][2, :, 1, :] = sqrt(2)*S[:, 2, :]; # S_itW^x
25     W[itW][3, :, 1, :] = sqrt(2)*S[:, 1, :]; # S_itW^y
26     W[itW][4, :, 2, :] = -t*sqrt(2)*S[:, 1, :]; # t*S_itW^x
27     W[itW][4, :, 3, :] = -t*sqrt(2)*S[:, 2, :]; # t*S_itW^y
28     W[itW][4, :, 4, :] = Id; # I
29 end
30 # last site
31 W[L] = zeros(Complex{Float64}, 4, 2, 1, 2); # ordering: left bottom right top
32 W[L][1, :, 1, :] = Id; # I
33 W[L][2, :, 1, :] = sqrt(2)*S[:, 2, :]; # S_L^x
34 W[L][3, :, 1, :] = sqrt(2)*S[:, 1, :]; # S_L^y
35
36 Eg_MPOF = reshape([1], (1, 1, 1));
37 for itL in (1:L)
38     global Eg_MPOF
39     Eg_MPOF = updateLeft(Eg_MPOF, 3, MPS[itL], W[itL], 4, MPS[itL]);
40 end
41
42 @printf("Ground state energy of Fermionic chain: %.4f\n", Eg_MPOF[1])
43
44 diff = Eg_MPO[1] - Eg_MPOF[1];
45 @printf("Difference between Eg_MPO and Eg_MPOF: %.4f\n", diff)

```

(iii) *MPO for one-particle eigenstates.* We obtain the ground state  $|\Psi_{\text{MPS}}\rangle$  of  $H_{\text{ff}}$  and construct the MPO for  $c_k$  as follows. The energies  $e_k, \varepsilon_k = \cos[\ell k\pi/(\mathcal{L}+1)]$  and their difference  $(e_k - \varepsilon_k)$  are plotted for  $k = 1, \dots, 25 (= \mathcal{L}/2)$ . We observe that the difference increases for increasing  $\mathcal{L}$  and fixing  $N_{\text{keep}}$  and decreases for increasing  $N_{\text{keep}}$  and fixing  $\mathcal{L}$ .

```

1 using LinearAlgebra
2 using Printf
3 using JLD2
4 using Plots
5
6 include("Tensor.jl");
7
8
9 # Iterative Diagonalization of Free Fermion
10 function diagFreeFermion(L, Nkeep)
11
12     global Hprev, Eg_Iter, MPS;
13
14     t = 0.5;
15     F, Z, Id = getLocalSpace("Fermion");
16
17     # MPS of the GS
18     MPS = Array{Any}(undef, 1, L);
19
20     # initialization
21     H0 = Id*0; # Hamiltonian for only the 1st site
22     A0 = getIdentity(1, 2, Id, 2); # 1st leg is dummy leg (vacuum)
23     Hnow = H0
24     D, V = eigen((Hnow+Hnow')/2)

```

```

25 MPS[1] = contract(A0,3,3,V,2,1)
26 Hprev = diagm(D)
27 Eg_Iter = nothing
28
29 for itL in (2:L)
30
31     # fermion annihilation operator at the current site
32     Fprev = updateLeft([],[],MPS[itL-1],F,3,MPS[itL-1])
33     Anow = getIdentity(Hprev,2,Id,2)
34     Hnow = updateLeft(Hprev,2,Anow,[],[],Anow)
35     # free fermion hopping
36     Hhop = t * updateLeft(Fprev,3,Anow,permutedims(F,(3,2,1)),3,Anow);
37     Hhop = Hhop + Hhop';
38     Hnow = Hnow + Hhop;
39     # diagonalize the current Hamiltonian
40     D,V = eigen((Hnow+Hnow')/2)
41     # sort eigenvalues & eigenvectors in the order of increasing
42     # eigenvalues
43     ids = sortperm(D)
44     D = D[ids]
45     V = V[:,ids]
46
47     if itL == L; Eg_Iter = minimum(D); end
48
49     # truncation threshold for energy
50     Etr = D[min(length(D),Nkeep)]
51     oks = (D .< Etr)
52     # true: to keep; false: not to keep
53     # keep all degenerate states up to tolerance
54
55     if itL < L
56         MPS[itL] = contract(Anow,3,3,V[:,oks],2,1)
57     else
58         MPS[itL] = contract(Anow,3,3,reshape(V[:,1],(size(V[:,1])[1],1)),2,1) #
59         # select GS at the last step
60     end
61     Hprev = diagm(D[oks])
62 end
63
64 return Eg_Iter
65
66 end
67
68
69
70 # MPO Method for Free Fermion
71 function mpoFreeFermion(L)
72
73     global Eg_MPOF, W
74
75     t = 0.5;
76     F,Z,Id = getLocalSpace("Fermion");
77
78     W = Array{Any}(undef,1,L); # MPO W
79     # first site
80     W[1] = zeros(1,2,4,2); # ordering: left bottom right top
81     W[1][1,.,2,.] = t*F[:,1,:]; # t*F'
82     W[1][1,.,3,.] = t*F[:,1,:]; # t*F
83     W[1][1,.,4,.] = Id; # I
84     # sites between first & last sites
85     for itW in (2:L-1)
86         W[itW] = zeros(4,2,4,2); # ordering: left bottom right top
87         W[itW][1,.,1,.] = Id; # I
88         W[itW][2,.,1,.] = F[:,1,:]; # F
89         W[itW][3,.,1,.] = F[:,1,:]; # F'
90         W[itW][4,.,2,.] = t*F[:,1,:]; # t*F'
91         W[itW][4,.,3,.] = t*F[:,1,:]; # t*F
92         W[itW][4,.,4,.] = Id; # I
93     end
94     # last site
95     W[L] = zeros(4,2,1,2); # ordering: left bottom right top
96     W[L][1,.,1,.] = Id; # I
97     W[L][2,.,1,.] = F[:,1,:]; # F
98     W[L][3,.,1,.] = F[:,1,:]; # F'
99

```

```

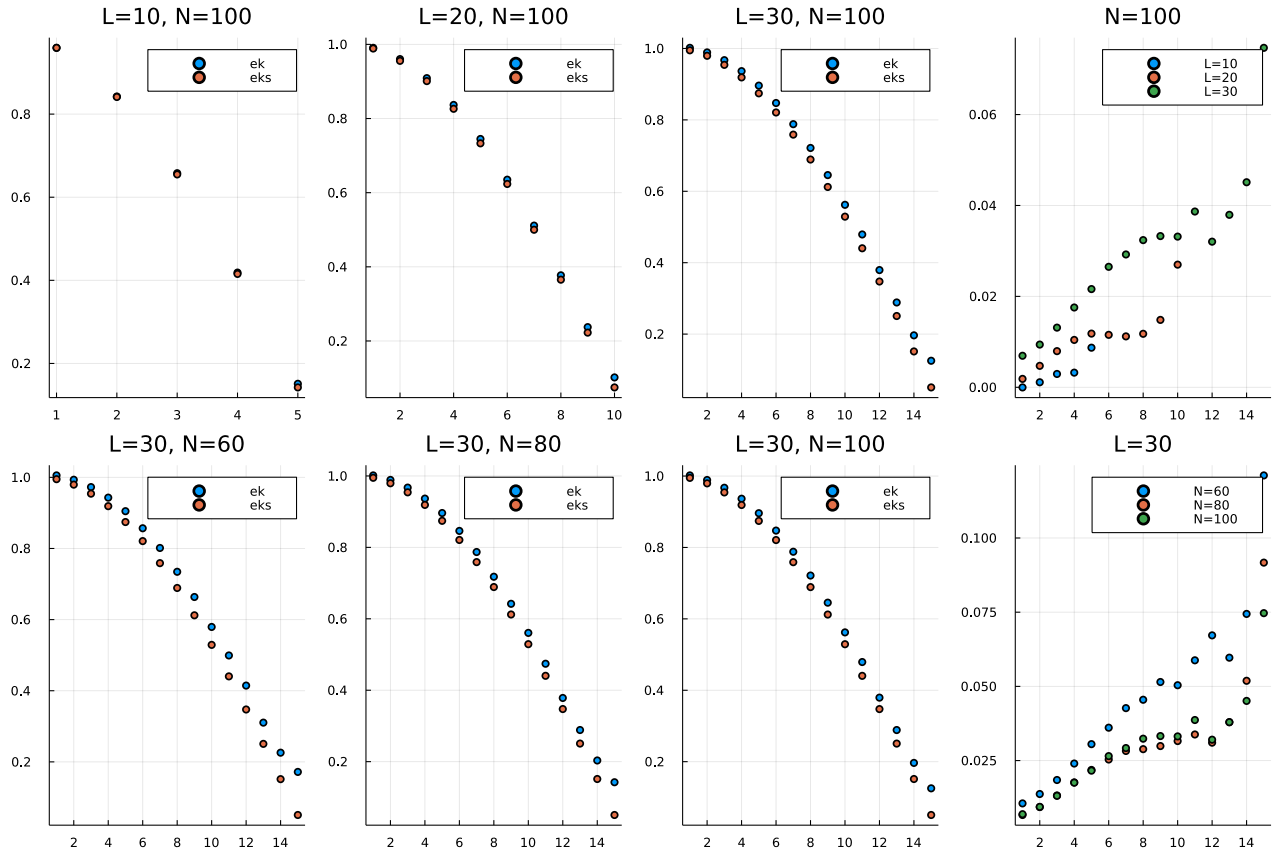
100 Eg_MPOF = reshape([1],(1,1,1));
101 for itL in (1:L)
102     Eg_MPOF = updateLeft(Eg_MPOF,3,MPS[itL],W[itL],4,MPS[itL]);
103 end
104
105 return Eg_MPOF[1]
106
107 end
108
109
110 # ek for Free Fermion
111 function ekFreeFermion(k,L)
112
113     global ckMPS, Egk
114
115     F,Z,Id = getLocalSpace("Fermion");
116
117     Wk = Array{Any}(undef,1,L); # MPO W
118     # first site
119     Wk[1] = zeros(1,2,2,2); # ordering: left bottom right top
120     Wk[1][1, :, 1, :] = sqrt(2/(L+1))*sin(1*k*pi/(L+1))*F[:,1,:];
121     Wk[1][1, :, 2, :] = Id;
122     # sites between first & last sites
123     for itW in (2:L-1)
124         Wk[itW] = zeros(2,2,2,2); # ordering: left bottom right top
125         Wk[itW][1, :, 1, :] = Z; # I
126         Wk[itW][2, :, 1, :] = sqrt(2/(L+1))*sin(itW*k*pi/(L+1))*F[:,1,:];
127         Wk[itW][2, :, 2, :] = Id;
128     end
129     # last site
130     Wk[L] = zeros(2,2,1,2); # ordering: left bottom right top
131     Wk[L][1, :, 1, :] = Z; # I
132     Wk[L][2, :, 1, :] = sqrt(2/(L+1))*sin(L*k*pi/(L+1))*F[:,1,:];
133
134     ckMPS = Array{Any}(undef,1,L);
135     Egk = reshape([1],(1,1,1));
136     for itL in (1:L)
137         ckMPS[itL] = contract(Wk[itL],4,4,MPS[itL],3,2,[1 4 2 3 5]);
138         ckMPS[itL] = reshape(ckMPS[itL],
139             (size(Wk[itL],1)*size(MPS[itL],1),
140             size(Wk[itL],2),
141             size(Wk[itL],3)*size(MPS[itL],3)));
142         Egk = updateLeft(Egk,3,ckMPS[itL],W[itL],4,ckMPS[itL]);
143     end
144
145     return Egk[1] - Eg_Iter
146
147 end
148
149
150 # make comparisons
151 L = 30
152 Nkeep = 100;
153 rangeL = 10:10:30;
154 rangeN = 60:20:100;
155
156 ekL = Array{Any}(undef,1,length(rangeL));
157 ekN = Array{Any}(undef,1,length(rangeN));
158
159 for itL in 1:length(rangeL)
160     Eg_Iter = diagFreeFermion(rangeL[itL],Nkeep);
161     Eg_MPOF = mpoFreeFermion(rangeL[itL]);
162     @printf("Eg_Iter - Eg_MPOF = %.4f\n", Eg_Iter - Eg_MPOF);
163     ekL[itL] = zeros(rangeL[itL]/2)
164     for itk in 1:rangeL[itL]/2
165         ekL[itL][itk] = ekFreeFermion(itk,rangeL[itL]);
166         @printf(" k = %i, ek - epsk = %.4f\n", itk,
167             ekL[itL][itk] - cos(itk*pi/(rangeL[itL]+1)))
168     end
169 end
170
171
172 for itN in 1:length(rangeN)
173     Eg_Iter = diagFreeFermion(L,rangeN[itN]);
174     Eg_MPOF = mpoFreeFermion(L);
175     @printf("Eg_Iter - Eg_MPOF = %.4f\n", Eg_Iter - Eg_MPOF);

```

```

176     ekN[itN] = zeros(L/2)
177     for itk in 1:L/2
178         ekN[itN][itk] = ekFreeFermion(itk,L);
179         @printf("  k = %i, ek - epsk = %.4f\n", itk,
180             ekN[itN][itk] - cos(itk*pi/(L+1)))
181     end
182 end
183
184
185 # plot the results
186 pL = Array{Any}(undef,1,length(ekL)+1);
187 pN = Array{Any}(undef,1,length(ekN)+1);
188 diffL = Array{Any}(undef,1,length(ekL)+1);
189 diffN = Array{Any}(undef,1,length(ekN)+1);
190
191 for itL = 1:length(ekL)
192     L = length(ekL[itL])*2; N = 100;
193     exact = cos.(collect(1:length(ekL[itL])).*pi ./ (length(ekL[itL])*2+1));
194     pL[itL] = scatter([1:length(ekL[itL]),1:length(ekL[itL])],
195         [ekL[itL],exact], labels=["ek" "eks"], title="L=$L, N=$N")
196     diffL[itL] = ekL[itL] - exact;
197 end
198 L = length(ekL[1])*2; N = 100;
199 pL[end] = scatter(1:length(ekL[1]),diffL[1],label="L=$L",title="N=$N")
200 for itL = 2:length(ekL)
201     L = length(ekL[itL])*2; N = 100;
202     scatter!(1:length(ekL[itL]),diffL[itL],label="L=$L",title="N=$N")
203 end
204
205 for itN = 1:length(ekN)
206     L = 30; N = rangeN[itN];
207     exact = cos.(collect(1:length(ekN[itN])).*pi ./ (length(ekN[itN])*2+1));
208     pN[itN] = scatter([1:length(ekN[itN]),1:length(ekN[itN])],
209         [ekN[itN],exact], labels=["ek" "eks"], title="L=$L, N=$N")
210     diffN[itN] = ekN[itN] - exact;
211 end
212 L = 30; N = rangeN[1];
213 pN[end] = scatter(1:length(ekN[1]),diffN[1],title="L=$L",label="N=$N")
214 for itN = 2:length(ekN)
215     L = 30; N = rangeN[itN];
216     scatter!(1:length(ekN[itN]),diffN[itN],title="L=$L",label="N=$N")
217 end
218
219 output = plot(pL..., pN..., layout = (2,4), size = (1200,800))
220 savefig(output,"output.pdf")

```




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[Total number of subtasks for T03: 17]

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