

[Tutorial T10.3] DMRG: error estimation (optional)

Author: Andreas Gleis

Exercise (a): Complete the function `twoSiteVariance_Ex.m`

There is a function `twoSiteVariance_Ex.m` which is placed in the same subdirectory together with this tutorial material. This function partially implements the calculation of the two-site variance as an error measure.

Complete the parts which are enclosed by the comments `TODO - Exercise 2`.

Heisenberg chain: error estimation

To test `twoSiteVariance_Ex.m` we consider a Heisenberg spin chain and calculate its ground-state. Its Hamiltonian is given by

$$H = \sum_{l=1}^{N-1} \vec{S}_l \vec{S}_{l+1}.$$

In the following, we will compare the two-site variance of the optimized GS obtained by DMRG3S and two-site DMRG for different bond dimensions.

```
clear

% system parameter
J = 1; % coupling strength
N = 40; % number of sites in a chain

% DMRG parameter
Nsweep = 10; % number of pairs of left+right sweeps

% magnitude of local spin
s = 1/2;
% Local operators
[S,I] = getLocalSpace('Spin',s);
```

We set up the MPO of the Heisenberg chain as given in the lecture:

```
% % MPO formulation of Hamiltonian
% Hamiltonian tensor for each chain site
Hloc = cell(5,5);
Hloc(:) = {zeros(size(I))};
Hloc{1,1} = I;
Hloc{2,1} = squeeze(S(:,1,:));
Hloc{3,1} = squeeze(S(:,2,:));
Hloc{4,1} = squeeze(S(:,3,:));
Hloc{end,2} = J*(Hloc{2,1}');
Hloc{end,3} = J*(Hloc{3,1}');
Hloc{end,4} = J*(Hloc{4,1}');
Hloc{end,end} = I;
```

```

Hloc = cell2mat(reshape(Hloc,[1 1 size(Hloc,1) size(Hloc,2)]));
Hloc = permute(Hloc,[3 1 4 2]); % leg order: left-bottom-right-top

% full chain
Hs = cell(1,N);
Hs(:) = {Hloc};
Hs{1} = Hs{1}(end,:,:,); % choose the last components of the left leg
Hs{end} = Hs{end}(:,:,1,:); % choose the first components of the right leg

```

Run the DMRG for different bond dimensions.

```

Nkeeps = [5,10,20,40,80,160]; % bond dimensions
var_2site = zeros(1,numel(Nkeeps));
var_3S = zeros(1,numel(Nkeeps));
for itK = 1:numel(Nkeeps)
    Nkeep = Nkeeps(itK);

    % first 2-site DMRG:
    [MGS_2site,~,~] = DMRG_2site(Hs,Nkeep,Nsweep);
    var_2site(itK) = twoSiteVariance_Ex(MGS_2site,Hs);

    % DMRG3S
    [MGS_3S,~,~] = DMRG_3S(Hs,Nkeep,Nsweep);
    var_3S(itK) = twoSiteVariance_Ex(MGS_3S,Hs);
end

```

```

Two-site DMRG: search for the ground state
# of sites = 40, Nkeep = 5, # of sweeps = 10 x 2
21-05-28 18:09:35 | Initialize with iterative diagonalization. Energy = -16.8593
21-05-28 18:09:35 | Sweep #1/20 (right -> left) : Energy = -17.48374
21-05-28 18:09:35 | Sweep #2/20 (left -> right) : Energy = -17.48719
21-05-28 18:09:35 | Sweep #3/20 (right -> left) : Energy = -17.4882
21-05-28 18:09:36 | Sweep #4/20 (left -> right) : Energy = -17.48858
21-05-28 18:09:36 | Sweep #5/20 (right -> left) : Energy = -17.48872
21-05-28 18:09:36 | Sweep #6/20 (left -> right) : Energy = -17.48877
21-05-28 18:09:36 | Sweep #7/20 (right -> left) : Energy = -17.4888
21-05-28 18:09:36 | Sweep #8/20 (left -> right) : Energy = -17.48881
21-05-28 18:09:36 | Sweep #9/20 (right -> left) : Energy = -17.48881
21-05-28 18:09:36 | Sweep #10/20 (left -> right) : Energy = -17.48882
21-05-28 18:09:36 | Sweep #11/20 (right -> left) : Energy = -17.48882
21-05-28 18:09:36 | Sweep #12/20 (left -> right) : Energy = -17.48882
21-05-28 18:09:36 | Sweep #13/20 (right -> left) : Energy = -17.48882
21-05-28 18:09:36 | Sweep #14/20 (left -> right) : Energy = -17.48882
21-05-28 18:09:36 | Sweep #15/20 (right -> left) : Energy = -17.48882
21-05-28 18:09:36 | Sweep #16/20 (left -> right) : Energy = -17.48882
21-05-28 18:09:36 | Sweep #17/20 (right -> left) : Energy = -17.48882
21-05-28 18:09:36 | Sweep #18/20 (left -> right) : Energy = -17.48882
21-05-28 18:09:36 | Sweep #19/20 (right -> left) : Energy = -17.48882
21-05-28 18:09:36 | Sweep #20/20 (left -> right) : Energy = -17.48882
Elapsed time: 1.065s, CPU time: 1.18s, Avg # of cores: 1.108
DMRG3S: search for the ground state
# of sites = 40, Nkeep = 5, # of sweeps = 10 x 2
21-05-28 18:09:36 | Initialize with iterative diagonalization. Energy = -16.8593
21-05-28 18:09:36 | Sweep #1/20 (right -> left) : Energy = -17.48149
21-05-28 18:09:37 | Sweep #2/20 (left -> right) : Energy = -17.48739
21-05-28 18:09:37 | Sweep #3/20 (right -> left) : Energy = -17.48862
21-05-28 18:09:37 | Sweep #4/20 (left -> right) : Energy = -17.48897
21-05-28 18:09:37 | Sweep #5/20 (right -> left) : Energy = -17.48908
21-05-28 18:09:37 | Sweep #6/20 (left -> right) : Energy = -17.48911

```

```

21-05-28 18:09:37 | Sweep #7/20 (right -> left) : Energy = -17.48911
21-05-28 18:09:37 | Sweep #8/20 (left -> right) : Energy = -17.48912
21-05-28 18:09:37 | Sweep #9/20 (right -> left) : Energy = -17.48912
21-05-28 18:09:37 | Sweep #10/20 (left -> right) : Energy = -17.48912
21-05-28 18:09:37 | Sweep #11/20 (right -> left) : Energy = -17.48912
21-05-28 18:09:37 | Sweep #12/20 (left -> right) : Energy = -17.48912
21-05-28 18:09:37 | Sweep #13/20 (right -> left) : Energy = -17.48912
21-05-28 18:09:37 | Sweep #14/20 (left -> right) : Energy = -17.48912
21-05-28 18:09:37 | Sweep #15/20 (right -> left) : Energy = -17.48912
21-05-28 18:09:37 | Sweep #16/20 (left -> right) : Energy = -17.48912
21-05-28 18:09:38 | Sweep #17/20 (right -> left) : Energy = -17.48912
21-05-28 18:09:38 | Sweep #18/20 (left -> right) : Energy = -17.48912
21-05-28 18:09:38 | Sweep #19/20 (right -> left) : Energy = -17.48912
21-05-28 18:09:38 | Sweep #20/20 (left -> right) : Energy = -17.48912
Elapsed time: 1.327s, CPU time: 1.62s, Avg # of cores: 1.22
Two-site DMRG: search for the ground state
# of sites = 40, Nkeep = 10, # of sweeps = 10 x 2
21-05-28 18:09:38 | Initialize with iterative diagonalization. Energy = -17.17619
21-05-28 18:09:38 | Sweep #1/20 (right -> left) : Energy = -17.5396
21-05-28 18:09:38 | Sweep #2/20 (left -> right) : Energy = -17.53968
21-05-28 18:09:38 | Sweep #3/20 (right -> left) : Energy = -17.53968
21-05-28 18:09:38 | Sweep #4/20 (left -> right) : Energy = -17.53968
21-05-28 18:09:38 | Sweep #5/20 (right -> left) : Energy = -17.53968
21-05-28 18:09:38 | Sweep #6/20 (left -> right) : Energy = -17.53968
21-05-28 18:09:38 | Sweep #7/20 (right -> left) : Energy = -17.53968
21-05-28 18:09:38 | Sweep #8/20 (left -> right) : Energy = -17.53968
21-05-28 18:09:38 | Sweep #9/20 (right -> left) : Energy = -17.53968
21-05-28 18:09:38 | Sweep #10/20 (left -> right) : Energy = -17.53968
21-05-28 18:09:38 | Sweep #11/20 (right -> left) : Energy = -17.53968
21-05-28 18:09:38 | Sweep #12/20 (left -> right) : Energy = -17.53968
21-05-28 18:09:38 | Sweep #13/20 (right -> left) : Energy = -17.53968
21-05-28 18:09:39 | Sweep #14/20 (left -> right) : Energy = -17.53968
21-05-28 18:09:39 | Sweep #15/20 (right -> left) : Energy = -17.53968
21-05-28 18:09:39 | Sweep #16/20 (left -> right) : Energy = -17.53968
21-05-28 18:09:39 | Sweep #17/20 (right -> left) : Energy = -17.53968
21-05-28 18:09:39 | Sweep #18/20 (left -> right) : Energy = -17.53968
21-05-28 18:09:39 | Sweep #19/20 (right -> left) : Energy = -17.53968
21-05-28 18:09:39 | Sweep #20/20 (left -> right) : Energy = -17.53968
Elapsed time: 1.113s, CPU time: 1.92s, Avg # of cores: 1.726
DMRG3S: search for the ground state
# of sites = 40, Nkeep = 10, # of sweeps = 10 x 2
21-05-28 18:09:39 | Initialize with iterative diagonalization. Energy = -17.17619
21-05-28 18:09:39 | Sweep #1/20 (right -> left) : Energy = -17.53856
21-05-28 18:09:39 | Sweep #2/20 (left -> right) : Energy = -17.53966
21-05-28 18:09:39 | Sweep #3/20 (right -> left) : Energy = -17.5397
21-05-28 18:09:39 | Sweep #4/20 (left -> right) : Energy = -17.5397
21-05-28 18:09:39 | Sweep #5/20 (right -> left) : Energy = -17.5397
21-05-28 18:09:39 | Sweep #6/20 (left -> right) : Energy = -17.5397
21-05-28 18:09:39 | Sweep #7/20 (right -> left) : Energy = -17.5397
21-05-28 18:09:39 | Sweep #8/20 (left -> right) : Energy = -17.5397
21-05-28 18:09:40 | Sweep #9/20 (right -> left) : Energy = -17.5397
21-05-28 18:09:40 | Sweep #10/20 (left -> right) : Energy = -17.5397
21-05-28 18:09:40 | Sweep #11/20 (right -> left) : Energy = -17.5397
21-05-28 18:09:40 | Sweep #12/20 (left -> right) : Energy = -17.5397
21-05-28 18:09:40 | Sweep #13/20 (right -> left) : Energy = -17.5397
21-05-28 18:09:40 | Sweep #14/20 (left -> right) : Energy = -17.5397
21-05-28 18:09:40 | Sweep #15/20 (right -> left) : Energy = -17.5397
21-05-28 18:09:40 | Sweep #16/20 (left -> right) : Energy = -17.5397
21-05-28 18:09:40 | Sweep #17/20 (right -> left) : Energy = -17.5397
21-05-28 18:09:40 | Sweep #18/20 (left -> right) : Energy = -17.5397
21-05-28 18:09:40 | Sweep #19/20 (right -> left) : Energy = -17.5397
21-05-28 18:09:40 | Sweep #20/20 (left -> right) : Energy = -17.5397
Elapsed time: 1.28s, CPU time: 1.91s, Avg # of cores: 1.492
Two-site DMRG: search for the ground state
# of sites = 40, Nkeep = 20, # of sweeps = 10 x 2

```

```

21-05-28 18:09:40 | Initialize with iterative diagonalization. Energy = -17.32798
21-05-28 18:09:40 | Sweep #1/20 (right -> left) : Energy = -17.54142
21-05-28 18:09:40 | Sweep #2/20 (left -> right) : Energy = -17.54145
21-05-28 18:09:41 | Sweep #3/20 (right -> left) : Energy = -17.54145
21-05-28 18:09:41 | Sweep #4/20 (left -> right) : Energy = -17.54145
21-05-28 18:09:41 | Sweep #5/20 (right -> left) : Energy = -17.54145
21-05-28 18:09:41 | Sweep #6/20 (left -> right) : Energy = -17.54145
21-05-28 18:09:41 | Sweep #7/20 (right -> left) : Energy = -17.54145
21-05-28 18:09:41 | Sweep #8/20 (left -> right) : Energy = -17.54145
21-05-28 18:09:41 | Sweep #9/20 (right -> left) : Energy = -17.54145
21-05-28 18:09:41 | Sweep #10/20 (left -> right) : Energy = -17.54145
21-05-28 18:09:42 | Sweep #11/20 (right -> left) : Energy = -17.54145
21-05-28 18:09:42 | Sweep #12/20 (left -> right) : Energy = -17.54145
21-05-28 18:09:42 | Sweep #13/20 (right -> left) : Energy = -17.54145
21-05-28 18:09:42 | Sweep #14/20 (left -> right) : Energy = -17.54145
21-05-28 18:09:42 | Sweep #15/20 (right -> left) : Energy = -17.54145
21-05-28 18:09:42 | Sweep #16/20 (left -> right) : Energy = -17.54145
21-05-28 18:09:42 | Sweep #17/20 (right -> left) : Energy = -17.54145
21-05-28 18:09:42 | Sweep #18/20 (left -> right) : Energy = -17.54145
21-05-28 18:09:42 | Sweep #19/20 (right -> left) : Energy = -17.54145
21-05-28 18:09:43 | Sweep #20/20 (left -> right) : Energy = -17.54145
Elapsed time: 2.337s, CPU time: 19.22s, Avg # of cores: 8.223
DMRG3S: search for the ground state
# of sites = 40, Nkeep = 20, # of sweeps = 10 x 2
21-05-28 18:09:43 | Initialize with iterative diagonalization. Energy = -17.32798
21-05-28 18:09:43 | Sweep #1/20 (right -> left) : Energy = -17.54141
21-05-28 18:09:43 | Sweep #2/20 (left -> right) : Energy = -17.54145
21-05-28 18:09:43 | Sweep #3/20 (right -> left) : Energy = -17.54145
21-05-28 18:09:43 | Sweep #4/20 (left -> right) : Energy = -17.54145
21-05-28 18:09:43 | Sweep #5/20 (right -> left) : Energy = -17.54145
21-05-28 18:09:43 | Sweep #6/20 (left -> right) : Energy = -17.54145
21-05-28 18:09:44 | Sweep #7/20 (right -> left) : Energy = -17.54145
21-05-28 18:09:44 | Sweep #8/20 (left -> right) : Energy = -17.54145
21-05-28 18:09:44 | Sweep #9/20 (right -> left) : Energy = -17.54145
21-05-28 18:09:44 | Sweep #10/20 (left -> right) : Energy = -17.54145
21-05-28 18:09:44 | Sweep #11/20 (right -> left) : Energy = -17.54145
21-05-28 18:09:44 | Sweep #12/20 (left -> right) : Energy = -17.54145
21-05-28 18:09:44 | Sweep #13/20 (right -> left) : Energy = -17.54145
21-05-28 18:09:44 | Sweep #14/20 (left -> right) : Energy = -17.54145
21-05-28 18:09:44 | Sweep #15/20 (right -> left) : Energy = -17.54145
21-05-28 18:09:44 | Sweep #16/20 (left -> right) : Energy = -17.54145
21-05-28 18:09:45 | Sweep #17/20 (right -> left) : Energy = -17.54145
21-05-28 18:09:45 | Sweep #18/20 (left -> right) : Energy = -17.54145
21-05-28 18:09:45 | Sweep #19/20 (right -> left) : Energy = -17.54145
21-05-28 18:09:45 | Sweep #20/20 (left -> right) : Energy = -17.54145
Elapsed time: 2.116s, CPU time: 14.64s, Avg # of cores: 6.919
Two-site DMRG: search for the ground state
# of sites = 40, Nkeep = 40, # of sweeps = 10 x 2
21-05-28 18:09:45 | Initialize with iterative diagonalization. Energy = -17.4161
21-05-28 18:09:45 | Sweep #1/20 (right -> left) : Energy = -17.54147
21-05-28 18:09:45 | Sweep #2/20 (left -> right) : Energy = -17.54147
21-05-28 18:09:45 | Sweep #3/20 (right -> left) : Energy = -17.54147
21-05-28 18:09:46 | Sweep #4/20 (left -> right) : Energy = -17.54147
21-05-28 18:09:46 | Sweep #5/20 (right -> left) : Energy = -17.54147
21-05-28 18:09:46 | Sweep #6/20 (left -> right) : Energy = -17.54147
21-05-28 18:09:46 | Sweep #7/20 (right -> left) : Energy = -17.54147
21-05-28 18:09:46 | Sweep #8/20 (left -> right) : Energy = -17.54147
21-05-28 18:09:47 | Sweep #9/20 (right -> left) : Energy = -17.54147
21-05-28 18:09:47 | Sweep #10/20 (left -> right) : Energy = -17.54147
21-05-28 18:09:47 | Sweep #11/20 (right -> left) : Energy = -17.54147
21-05-28 18:09:47 | Sweep #12/20 (left -> right) : Energy = -17.54147
21-05-28 18:09:47 | Sweep #13/20 (right -> left) : Energy = -17.54147
21-05-28 18:09:47 | Sweep #14/20 (left -> right) : Energy = -17.54147
21-05-28 18:09:48 | Sweep #15/20 (right -> left) : Energy = -17.54147
21-05-28 18:09:48 | Sweep #16/20 (left -> right) : Energy = -17.54147

```

```

21-05-28 18:09:48 | Sweep #17/20 (right -> left) : Energy = -17.54147
21-05-28 18:09:48 | Sweep #18/20 (left -> right) : Energy = -17.54147
21-05-28 18:09:48 | Sweep #19/20 (right -> left) : Energy = -17.54147
21-05-28 18:09:48 | Sweep #20/20 (left -> right) : Energy = -17.54147
Elapsed time: 3.579s, CPU time: 30.17s, Avg # of cores: 8.43
DMRG3S: search for the ground state
# of sites = 40, Nkeep = 40, # of sweeps = 10 x 2
21-05-28 18:09:49 | Initialize with iterative diagonalization. Energy = -17.4161
21-05-28 18:09:49 | Sweep #1/20 (right -> left) : Energy = -17.54147
21-05-28 18:09:49 | Sweep #2/20 (left -> right) : Energy = -17.54147
21-05-28 18:09:49 | Sweep #3/20 (right -> left) : Energy = -17.54147
21-05-28 18:09:49 | Sweep #4/20 (left -> right) : Energy = -17.54147
21-05-28 18:09:50 | Sweep #5/20 (right -> left) : Energy = -17.54147
21-05-28 18:09:50 | Sweep #6/20 (left -> right) : Energy = -17.54147
21-05-28 18:09:50 | Sweep #7/20 (right -> left) : Energy = -17.54147
21-05-28 18:09:50 | Sweep #8/20 (left -> right) : Energy = -17.54147
21-05-28 18:09:50 | Sweep #9/20 (right -> left) : Energy = -17.54147
21-05-28 18:09:50 | Sweep #10/20 (left -> right) : Energy = -17.54147
21-05-28 18:09:51 | Sweep #11/20 (right -> left) : Energy = -17.54147
21-05-28 18:09:51 | Sweep #12/20 (left -> right) : Energy = -17.54147
21-05-28 18:09:51 | Sweep #13/20 (right -> left) : Energy = -17.54147
21-05-28 18:09:51 | Sweep #14/20 (left -> right) : Energy = -17.54147
21-05-28 18:09:51 | Sweep #15/20 (right -> left) : Energy = -17.54147
21-05-28 18:09:51 | Sweep #16/20 (left -> right) : Energy = -17.54147
21-05-28 18:09:52 | Sweep #17/20 (right -> left) : Energy = -17.54147
21-05-28 18:09:52 | Sweep #18/20 (left -> right) : Energy = -17.54147
21-05-28 18:09:52 | Sweep #19/20 (right -> left) : Energy = -17.54147
21-05-28 18:09:52 | Sweep #20/20 (left -> right) : Energy = -17.54147
Elapsed time: 3.625s, CPU time: 31.9s, Avg # of cores: 8.801
Two-site DMRG: search for the ground state
# of sites = 40, Nkeep = 80, # of sweeps = 10 x 2
21-05-28 18:09:53 | Initialize with iterative diagonalization. Energy = -17.5012
21-05-28 18:09:53 | Sweep #1/20 (right -> left) : Energy = -17.54147
21-05-28 18:09:53 | Sweep #2/20 (left -> right) : Energy = -17.54147
21-05-28 18:09:54 | Sweep #3/20 (right -> left) : Energy = -17.54147
21-05-28 18:09:54 | Sweep #4/20 (left -> right) : Energy = -17.54147
21-05-28 18:09:55 | Sweep #5/20 (right -> left) : Energy = -17.54147
21-05-28 18:09:55 | Sweep #6/20 (left -> right) : Energy = -17.54147
21-05-28 18:09:55 | Sweep #7/20 (right -> left) : Energy = -17.54147
21-05-28 18:09:56 | Sweep #8/20 (left -> right) : Energy = -17.54147
21-05-28 18:09:56 | Sweep #9/20 (right -> left) : Energy = -17.54147
21-05-28 18:09:56 | Sweep #10/20 (left -> right) : Energy = -17.54147
21-05-28 18:09:57 | Sweep #11/20 (right -> left) : Energy = -17.54147
21-05-28 18:09:57 | Sweep #12/20 (left -> right) : Energy = -17.54147
21-05-28 18:09:58 | Sweep #13/20 (right -> left) : Energy = -17.54147
21-05-28 18:09:58 | Sweep #14/20 (left -> right) : Energy = -17.54147
21-05-28 18:09:58 | Sweep #15/20 (right -> left) : Energy = -17.54147
21-05-28 18:09:59 | Sweep #16/20 (left -> right) : Energy = -17.54147
21-05-28 18:09:59 | Sweep #17/20 (right -> left) : Energy = -17.54147
21-05-28 18:10:00 | Sweep #18/20 (left -> right) : Energy = -17.54147
21-05-28 18:10:00 | Sweep #19/20 (right -> left) : Energy = -17.54147
21-05-28 18:10:01 | Sweep #20/20 (left -> right) : Energy = -17.54147
Elapsed time: 8.33s, CPU time: 66s, Avg # of cores: 7.923
DMRG3S: search for the ground state
# of sites = 40, Nkeep = 80, # of sweeps = 10 x 2
21-05-28 18:10:01 | Initialize with iterative diagonalization. Energy = -17.5012
21-05-28 18:10:02 | Sweep #1/20 (right -> left) : Energy = -17.54147
21-05-28 18:10:02 | Sweep #2/20 (left -> right) : Energy = -17.54147
21-05-28 18:10:02 | Sweep #3/20 (right -> left) : Energy = -17.54147
21-05-28 18:10:03 | Sweep #4/20 (left -> right) : Energy = -17.54147
21-05-28 18:10:03 | Sweep #5/20 (right -> left) : Energy = -17.54147
21-05-28 18:10:04 | Sweep #6/20 (left -> right) : Energy = -17.54147
21-05-28 18:10:04 | Sweep #7/20 (right -> left) : Energy = -17.54147
21-05-28 18:10:04 | Sweep #8/20 (left -> right) : Energy = -17.54147
21-05-28 18:10:05 | Sweep #9/20 (right -> left) : Energy = -17.54147

```

```

21-05-28 18:10:05 | Sweep #10/20 (left -> right) : Energy = -17.54147
21-05-28 18:10:05 | Sweep #11/20 (right -> left) : Energy = -17.54147
21-05-28 18:10:06 | Sweep #12/20 (left -> right) : Energy = -17.54147
21-05-28 18:10:06 | Sweep #13/20 (right -> left) : Energy = -17.54147
21-05-28 18:10:07 | Sweep #14/20 (left -> right) : Energy = -17.54147
21-05-28 18:10:07 | Sweep #15/20 (right -> left) : Energy = -17.54147
21-05-28 18:10:07 | Sweep #16/20 (left -> right) : Energy = -17.54147
21-05-28 18:10:08 | Sweep #17/20 (right -> left) : Energy = -17.54147
21-05-28 18:10:08 | Sweep #18/20 (left -> right) : Energy = -17.54147
21-05-28 18:10:08 | Sweep #19/20 (right -> left) : Energy = -17.54147
21-05-28 18:10:09 | Sweep #20/20 (left -> right) : Energy = -17.54147
Elapsed time: 7.739s, CPU time: 63.06s, Avg # of cores: 8.148
Two-site DMRG: search for the ground state
# of sites = 40, Nkeep = 160, # of sweeps = 10 x 2
21-05-28 18:10:10 | Initialize with iterative diagonalization. Energy = -17.51978
21-05-28 18:10:12 | Sweep #1/20 (right -> left) : Energy = -17.54147
21-05-28 18:10:13 | Sweep #2/20 (left -> right) : Energy = -17.54147
21-05-28 18:10:15 | Sweep #3/20 (right -> left) : Energy = -17.54147
21-05-28 18:10:16 | Sweep #4/20 (left -> right) : Energy = -17.54147
21-05-28 18:10:17 | Sweep #5/20 (right -> left) : Energy = -17.54147
21-05-28 18:10:19 | Sweep #6/20 (left -> right) : Energy = -17.54147
21-05-28 18:10:20 | Sweep #7/20 (right -> left) : Energy = -17.54147
21-05-28 18:10:21 | Sweep #8/20 (left -> right) : Energy = -17.54147
21-05-28 18:10:23 | Sweep #9/20 (right -> left) : Energy = -17.54147
21-05-28 18:10:24 | Sweep #10/20 (left -> right) : Energy = -17.54147
21-05-28 18:10:25 | Sweep #11/20 (right -> left) : Energy = -17.54147
21-05-28 18:10:27 | Sweep #12/20 (left -> right) : Energy = -17.54147
21-05-28 18:10:28 | Sweep #13/20 (right -> left) : Energy = -17.54147
21-05-28 18:10:29 | Sweep #14/20 (left -> right) : Energy = -17.54147
21-05-28 18:10:31 | Sweep #15/20 (right -> left) : Energy = -17.54147
21-05-28 18:10:32 | Sweep #16/20 (left -> right) : Energy = -17.54147
21-05-28 18:10:33 | Sweep #17/20 (right -> left) : Energy = -17.54147
21-05-28 18:10:35 | Sweep #18/20 (left -> right) : Energy = -17.54147
21-05-28 18:10:36 | Sweep #19/20 (right -> left) : Energy = -17.54147
21-05-28 18:10:37 | Sweep #20/20 (left -> right) : Energy = -17.54147
Elapsed time: 28.55s, CPU time: 187.7s, Avg # of cores: 6.573
DMRG3S: search for the ground state
# of sites = 40, Nkeep = 160, # of sweeps = 10 x 2
21-05-28 18:10:40 | Initialize with iterative diagonalization. Energy = -17.51978
21-05-28 18:10:41 | Sweep #1/20 (right -> left) : Energy = -17.54147
21-05-28 18:10:42 | Sweep #2/20 (left -> right) : Energy = -17.54147
21-05-28 18:10:43 | Sweep #3/20 (right -> left) : Energy = -17.54147
21-05-28 18:10:45 | Sweep #4/20 (left -> right) : Energy = -17.54147
21-05-28 18:10:46 | Sweep #5/20 (right -> left) : Energy = -17.54147
21-05-28 18:10:47 | Sweep #6/20 (left -> right) : Energy = -17.54147
21-05-28 18:10:48 | Sweep #7/20 (right -> left) : Energy = -17.54147
21-05-28 18:10:49 | Sweep #8/20 (left -> right) : Energy = -17.54147
21-05-28 18:10:50 | Sweep #9/20 (right -> left) : Energy = -17.54147
21-05-28 18:10:51 | Sweep #10/20 (left -> right) : Energy = -17.54147
21-05-28 18:10:52 | Sweep #11/20 (right -> left) : Energy = -17.54147
21-05-28 18:10:53 | Sweep #12/20 (left -> right) : Energy = -17.54147
21-05-28 18:10:54 | Sweep #13/20 (right -> left) : Energy = -17.54147
21-05-28 18:10:55 | Sweep #14/20 (left -> right) : Energy = -17.54147
21-05-28 18:10:56 | Sweep #15/20 (right -> left) : Energy = -17.54147
21-05-28 18:10:57 | Sweep #16/20 (left -> right) : Energy = -17.54147
21-05-28 18:10:58 | Sweep #17/20 (right -> left) : Energy = -17.54147
21-05-28 18:10:59 | Sweep #18/20 (left -> right) : Energy = -17.54147
21-05-28 18:11:00 | Sweep #19/20 (right -> left) : Energy = -17.54147
21-05-28 18:11:01 | Sweep #20/20 (left -> right) : Energy = -17.54147
Elapsed time: 22.93s, CPU time: 154.1s, Avg # of cores: 6.719

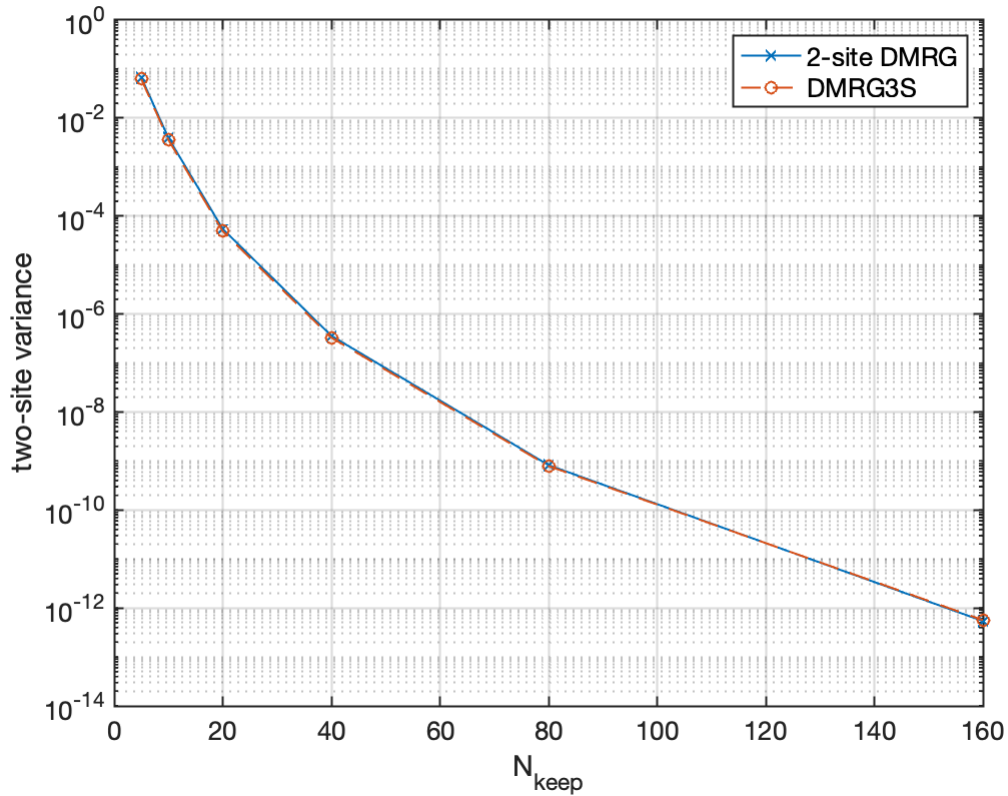
```

Plot how the two-site variance decreases with the bond dimension:

```

figure;
semilogy(Nkeeps,var_2site,'-x','LineWidth',1);
hold on;
semilogy(Nkeeps,var_3S,'--o','LineWidth',1);
set(gca,'FontSize',13,'LineWidth',1);
xlim([0 max(Nkeeps)]);
grid on;
legend({'2-site DMRG','DMRG3S'},'FontSize',13)
xlabel('N_{keep}');
ylabel('two-site variance');
hold off;

```



As expected, the variance decreases with N_{keep} . Two-site DMRG and DMRG3S yield almost identical variances. Note however that DMRG3S is only marginally faster for $s = 1/2$ than 2-site DMRG. This is because of the small physical dimension $d = 2$. If s is increased, d increases and the DMRG3S eventually becomes faster. However, calculations also become quite a bit heavier. But if your computer is able to handle it, give larger s a try!