[Solution] iTEBD: Ground state search

Author: Seung-Sup Lee

Solution to Exercise (a): Complete the function for Vidal's original iTEBD

Check out the funciton `iTEBD_GS_Vidal.m` under the DMRG sub-directory. Compare with your implementation of `iTEBD_GS_Vidal_Ex.m`!

Solution to Exercise (b): Check the energy convergence

In the demonstration, we use the following choice of parameters:

```
clear

% iTEBD parameters
Nkeep = 30;
tau_ini = 1; % initial imaginary time step size
tau_fin = 1e-6; % final imaginary time step size
Nstep = 2e3;
```

In this solution, I will see how iTEBD's performance changes with chaging (i) `tau_fin`, (ii) `Nstep`, or (iii) `Nkeep`. We use the same random MPS as the initial state, for fair comparison.

```
% Local operators
[S,I] = getLocalSpace('Spin',1);
% Heisenberg interaction as two-site gate S*S'
H = contract(S,3,3,permute(conj(S),[2 1 3]),3,3);

% Initialize with random Lambda and Gamma
Lambda_init = cell(1,2);
Gamma_init = cell(1,2);
for itn = (1:numel(Lambda_init))
    Lambda_init{itn} = rand(Nkeep,1);
    Gamma_init{itn} = rand(Nkeep,Nkeep,size(I,2));
end

% "numerically exact" value by White & Huse
Eexact = -1.401484039;
```

First, let's see the dependence of `tau_fin`.

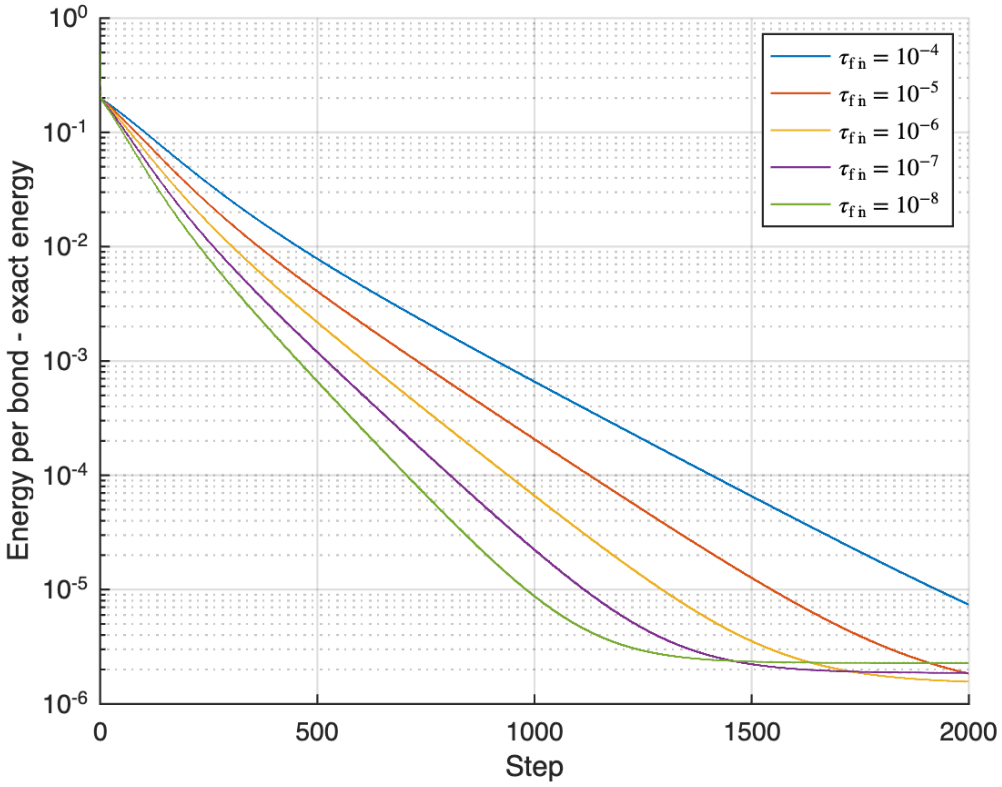
```
tau_fins = 10.^(-4:-1:-8);
Eiters = cell(size(tau_fins));

for itt = (1:numel(Eiters))
    taus = tau_ini*((tau_fins(itt)/tau_ini).^linspace(0,1,Nstep));
    % iTEBD ground state search
    [~,~,Eiters{itt}] = iTEBD_GS_Vidal(Lambda_init,Gamma_init,H,Nkeep,taus);
```

```
end
```

```
22-10-02 12:17:20 | iTEBD ground state search: Bond dim. Nkeep = 30, # of imag. time steps = 2000
22-10-02 12:17:23 | #500/2000, E = -1.3935978
22-10-02 12:17:26 | #1000/2000, E = -1.4008203
22-10-02 12:17:28 | #1500/2000, E = -1.4014181
22-10-02 12:17:31 | #2000/2000, E = -1.4014766
Elapsed time: 11.45s, CPU time: 117.7s, Avg # of cores: 10.28
22-10-02 12:17:31 | Memory usage : 2.58GiB
22-10-02 12:17:31 | iTEBD ground state search: Bond dim. Nkeep = 30, # of imag. time steps = 2000
22-10-02 12:17:34 | #500/2000, E = -1.3973875
22-10-02 12:17:37 | #1000/2000, E = -1.4012757
22-10-02 12:17:40 | #1500/2000, E = -1.4014713
22-10-02 12:17:42 | #2000/2000, E = -1.4014822
Elapsed time: 11.14s, CPU time: 113.2s, Avg # of cores: 10.16
22-10-02 12:17:42 | Memory usage : 2.59GiB
22-10-02 12:17:42 | iTEBD ground state search: Bond dim. Nkeep = 30, # of imag. time steps = 2000
22-10-02 12:17:45 | #500/2000, E = -1.3992815
22-10-02 12:17:48 | #1000/2000, E = -1.4014172
22-10-02 12:17:50 | #1500/2000, E = -1.4014805
22-10-02 12:17:53 | #2000/2000, E = -1.4014825
Elapsed time: 10.61s, CPU time: 108.8s, Avg # of cores: 10.25
22-10-02 12:17:53 | Memory usage : 2.60GiB
22-10-02 12:17:53 | iTEBD ground state search: Bond dim. Nkeep = 30, # of imag. time steps = 2000
22-10-02 12:17:56 | #500/2000, E = -1.4002749
22-10-02 12:17:58 | #1000/2000, E = -1.4014615
22-10-02 12:18:01 | #1500/2000, E = -1.4014818
22-10-02 12:18:04 | #2000/2000, E = -1.4014822
Elapsed time: 10.89s, CPU time: 111.8s, Avg # of cores: 10.26
22-10-02 12:18:04 | Memory usage : 2.60GiB
22-10-02 12:18:04 | iTEBD ground state search: Bond dim. Nkeep = 30, # of imag. time steps = 2000
22-10-02 12:18:07 | #500/2000, E = -1.4008117
22-10-02 12:18:09 | #1000/2000, E = -1.4014752
22-10-02 12:18:12 | #1500/2000, E = -1.4014817
22-10-02 12:18:15 | #2000/2000, E = -1.4014818
Elapsed time: 11.34s, CPU time: 115.3s, Avg # of cores: 10.17
22-10-02 12:18:15 | Memory usage : 2.60GiB
```

```
figure;
legs = cell(size(Eiters));
hold on;
for itt = (1:numel(Eiters))
    Eiter2 = reshape(permute(Eiters{itt},[2 1 3]), ...
        [size(Eiters{itt},2)*size(Eiters{itt},1) size(Eiters{itt},3)]);
    plot((1:size(Eiter2,1)).'/2,mean(Eiter2,2)-Eexact,'LineWidth',1);
    legs{itt} = ['$\tau_\mathrm{fin} = 10^{', ...
        sprintf('%i',log10(tau_fins(itt))),'}$'];
end
hold off;
set(gca,'YScale','log','LineWidth',1,'FontSize',13);
xlabel('Step');
ylabel('Energy per bond - exact energy');
legend(legs{:},'Interpreter','latex');
grid on;
```



We find that for the largest `tau_fin`'s (10^{-4} and 10^{-5}) the energy has not fully converged. It is because larger step sizes in the last iterations lead to larger Trotterization error. For smaller `tau_fin`'s (10^{-7} and 10^{-8}) , the energy approaches faster, but the final value is larger than that for 10^{-6}. It is because the total imaginary time interval is smaller than that for 10^{-6}:

```
disp(sum(tau_ini*((tau_fins(3)/tau_ini).^linspace(0,1,Nstep)))); % 1e-6
```

```
145.1929
```

```
disp(sum(tau_ini*((tau_fins(5)/tau_ini).^linspace(0,1,Nstep)))); % 1e-8
```

```
109.0201
```

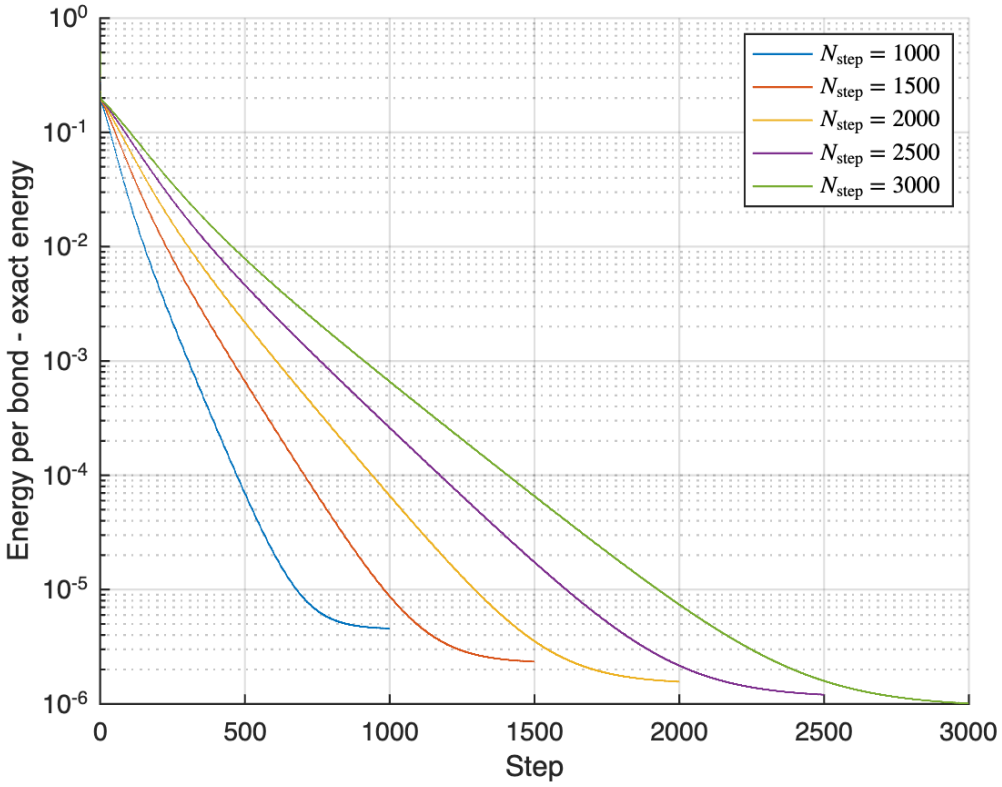
How about the dependence of `Nstep`?

```
Nsteps = (1e3:500:3e3);
Eiters = cell(size(Nsteps));

for itt = (1:numel(Eiters))
    taus = tau_ini*((tau_fin/tau_ini).^linspace(0,1,Nsteps(itt)));
    % iTEBD ground state search
    [~,~,Eiters{itt}] = iTEBD_GS_Vidal(Lambda_init,Gamma_init,H,Nkeep,taus);
end
```

```
22-10-02 12:18:16 | iTEBD ground state search: Bond dim. Nkeep = 30, # of imag. time steps = 1000
22-10-02 12:18:19 | #500/1000, E = -1.4014133
22-10-02 12:18:22 | #1000/1000, E = -1.4014795
Elapsed time: 6.371s, CPU time: 63.37s, Avg # of cores: 9.946
22-10-02 12:18:22 | Memory usage : 2.61GiB
22-10-02 12:18:22 | iTEBD ground state search: Bond dim. Nkeep = 30, # of imag. time steps = 1500
22-10-02 12:18:25 | #500/1500, E = -1.4008122
22-10-02 12:18:28 | #1000/1500, E = -1.4014752
22-10-02 12:18:31 | #1500/1500, E = -1.4014817
Elapsed time: 8.948s, CPU time: 91.27s, Avg # of cores: 10.2
22-10-02 12:18:31 | Memory usage : 2.61GiB
22-10-02 12:18:31 | iTEBD ground state search: Bond dim. Nkeep = 30, # of imag. time steps = 2000
22-10-02 12:18:34 | #500/2000, E = -1.3992815
22-10-02 12:18:37 | #1000/2000, E = -1.4014172
22-10-02 12:18:40 | #1500/2000, E = -1.4014805
22-10-02 12:18:42 | #2000/2000, E = -1.4014825
Elapsed time: 11.27s, CPU time: 116.1s, Avg # of cores: 10.31
22-10-02 12:18:43 | Memory usage : 2.62GiB
22-10-02 12:18:43 | iTEBD ground state search: Bond dim. Nkeep = 30, # of imag. time steps = 2500
22-10-02 12:18:45 | #500/2500, E = -1.3968282
22-10-02 12:18:48 | #1000/2500, E = -1.4012216
22-10-02 12:18:51 | #1500/2500, E = -1.4014666
22-10-02 12:18:53 | #2000/2500, E = -1.4014819
22-10-02 12:18:56 | #2500/2500, E = -1.4014828
Elapsed time: 13.69s, CPU time: 141.9s, Avg # of cores: 10.37
22-10-02 12:18:56 | Memory usage : 2.62GiB
22-10-02 12:18:56 | iTEBD ground state search: Bond dim. Nkeep = 30, # of imag. time steps = 3000
22-10-02 12:18:59 | #500/3000, E = -1.3935942
22-10-02 12:19:02 | #1000/3000, E = -1.4008197
22-10-02 12:19:04 | #1500/3000, E = -1.401418
22-10-02 12:19:07 | #2000/3000, E = -1.4014766
22-10-02 12:19:10 | #2500/3000, E = -1.4014824
22-10-02 12:19:12 | #3000/3000, E = -1.401483
Elapsed time: 16.04s, CPU time: 166.2s, Avg # of cores: 10.36
22-10-02 12:19:12 | Memory usage : 2.62GiB
```

```
figure;
legs = cell(size(Eiters));
hold on;
for itt = (1:numel(Eiters))
    Eiter2 = reshape(permute(Eiters{itt},[2 1 3]), ...
        [size(Eiters{itt},2)*size(Eiters{itt},1) size(Eiters{itt},3)]);
    plot((1:size(Eiter2,1)).'/2,mean(Eiter2,2)-Eexact,'LineWidth',1);
    legs{itt} = ['$N_\mathrm{step} = ',sprintf('%i',Nsteps(itt)),'$'];
end
hold off;
set(gca,'YScale','log','LineWidth',1,'FontSize',13);
xlabel('Step');
ylabel('Energy per bond - exact energy');
legend(legs{:},'Interpreter','latex');
grid on;
```



For smaller `Nstep`'s, the energy approaches faster, but the final value is larger than that for the largest `Nstep` (= 3000). It is because the total imaginary time interval is smaller.

As the last part of this analysis, we change `Nkeep`.

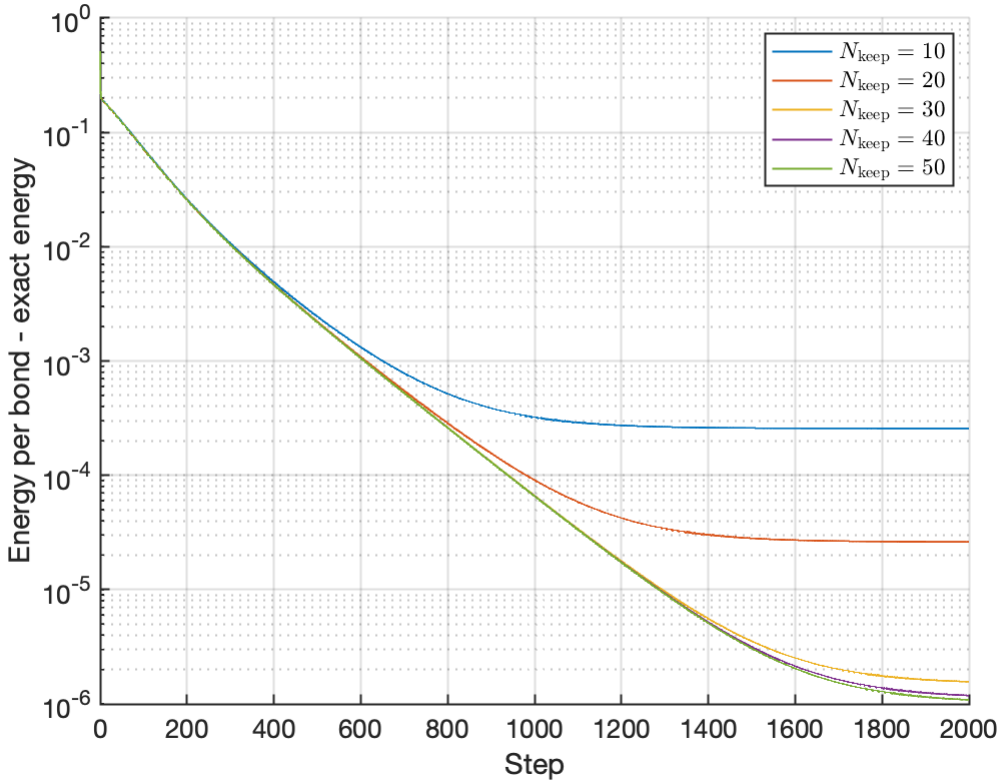
```
Nkeeps = (10:10:50);
Eiters = cell(size(Nkeeps));
taus = tau_ini*((tau_fin/tau_ini).^linspace(0,1,Nstep));

for itt = (1:numel(Eiters))
    % iTEBD ground state search
    [Lambda,Gamma,Eiters{itt}] = iTEBD_GS_Vidal(Lambda_init,Gamma_init,H,Nkeeps(itt),ta
end
```

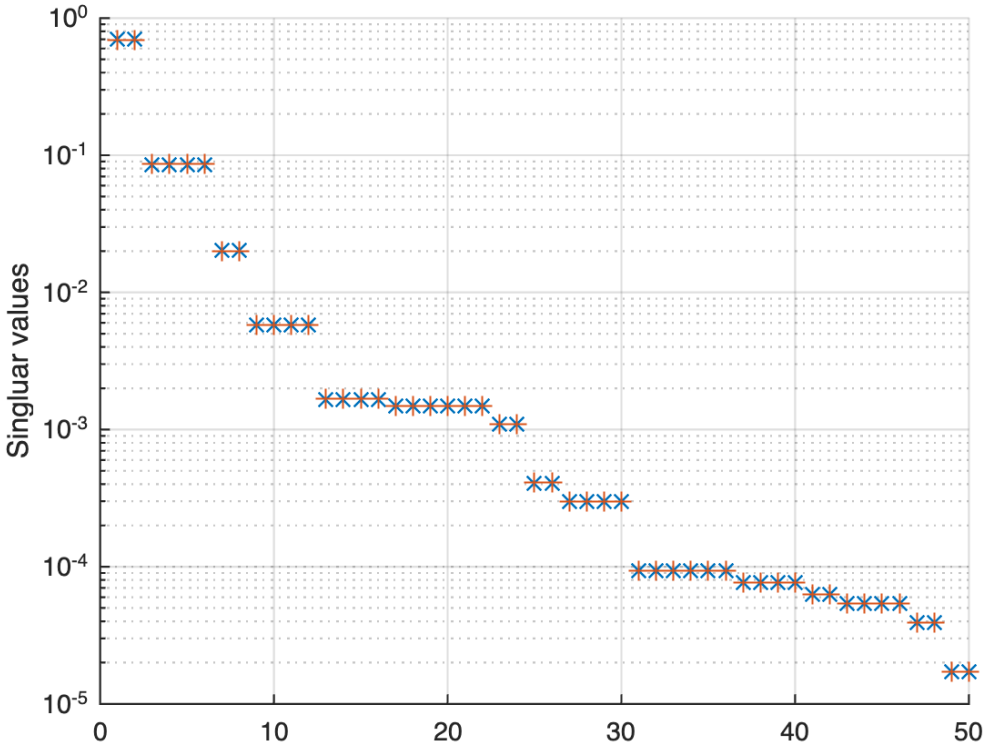
```
22-10-02 12:21:02 | iTEBD ground state search: Bond dim. Nkeep = 10, # of imag. time steps = 2000
22-10-02 12:21:03 | #500/2000, E = -1.3990145
22-10-02 12:21:04 | #1000/2000, E = -1.4011613
22-10-02 12:21:05 | #1500/2000, E = -1.401225
22-10-02 12:21:06 | #2000/2000, E = -1.401227
Elapsed time: 4.371s, CPU time: 5.8s, Avg # of cores: 1.327
22-10-02 12:21:06 | Memory usage : 2.78GiB
22-10-02 12:21:06 | iTEBD ground state search: Bond dim. Nkeep = 20, # of imag. time steps = 2000
22-10-02 12:21:08 | #500/2000, E = -1.3992544
22-10-02 12:21:10 | #1000/2000, E = -1.4013925
22-10-02 12:21:11 | #1500/2000, E = -1.4014559
22-10-02 12:21:13 | #2000/2000, E = -1.4014579
Elapsed time: 6.523s, CPU time: 52.98s, Avg # of cores: 8.123
22-10-02 12:21:13 | Memory usage : 2.79GiB
```

```
22-10-02 12:21:13 | iTEBD ground state search: Bond dim. Nkeep = 30, # of imag. time steps = 2000
22-10-02 12:21:16 | #500/2000, E = -1.3992815
22-10-02 12:21:18 | #1000/2000, E = -1.4014172
22-10-02 12:21:21 | #1500/2000, E = -1.4014805
22-10-02 12:21:23 | #2000/2000, E = -1.4014825
Elapsed time: 10.63s, CPU time: 109.3s, Avg # of cores: 10.28
22-10-02 12:21:23 | Memory usage : 2.79GiB
22-10-02 12:21:23 | iTEBD ground state search: Bond dim. Nkeep = 40, # of imag. time steps = 2000
22-10-02 12:21:27 | #500/2000, E = -1.3992819
22-10-02 12:21:30 | #1000/2000, E = -1.4014176
22-10-02 12:21:33 | #1500/2000, E = -1.4014809
22-10-02 12:21:37 | #2000/2000, E = -1.4014829
Elapsed time: 13.03s, CPU time: 130s, Avg # of cores: 9.976
22-10-02 12:21:37 | Memory usage : 2.79GiB
22-10-02 12:21:37 | iTEBD ground state search: Bond dim. Nkeep = 50, # of imag. time steps = 2000
22-10-02 12:21:41 | #500/2000, E = -1.399282
22-10-02 12:21:46 | #1000/2000, E = -1.4014177
22-10-02 12:21:51 | #1500/2000, E = -1.401481
22-10-02 12:21:55 | #2000/2000, E = -1.401483
Elapsed time: 18.8s, CPU time: 206.7s, Avg # of cores: 11
22-10-02 12:21:55 | Memory usage : 2.80GiB
```

```
figure;
legs = cell(size(Eiters));
hold on;
for itt = (1:numel(Eiters))
    Eiter2 = reshape(permute(Eiters{itt},[2 1 3]), ...
        [size(Eiters{itt},2)*size(Eiters{itt},1) size(Eiters{itt},3)]);
    plot((1:size(Eiter2,1)).'/2,mean(Eiter2,2)-Eexact,'LineWidth',1);
    legs{itt} = ['$N_\mathrm{keep} = ',sprintf('%i',Nkeeps(itt)),'$'];
end
hold off;
set(gca,'YScale','log','LineWidth',1,'FontSize',13);
xlabel('Step');
ylabel('Energy per bond - exact energy');
legend(legs{:},'Interpreter','latex');
grid on;
```




```
figure;
hold on;
plot((1:numel(Lambda{1})).',Lambda{1},'x','LineWidth',1,'MarkerSize',10);
plot((1:numel(Lambda{2})).',Lambda{2},'+','LineWidth',1,'MarkerSize',10);
hold off;
set(gca,'YScale','log','LineWidth',1,'FontSize',13);
ylabel('Singluar values');
grid on;
```



We find that the energy gets lower as Nkeep increases. The differences in the final energy values are due to the contibution from small singular values and the corresponding singular vectors (that would be discarded if Nkeep is smaller).