Problem 3. Tight-binding chain

First, construct MPO.

```matlab
function Hs = tb_chain_MPO(L, t)
    id = eye(2);
    c  = [0 1; 0 0];      % annihilation operator

    Hs = cell(1,L);

    for i = 1:L
        if i < L
            tl = t(i);
        else
            tl = 0;
        end

        W = zeros(2,2,4,4);

        W(:, :, 1, 1) = id;
        W(:, :, 2, 1) = c;
        W(:, :, 3, 1) = c';
        W(:, :, 4, 2) = -tl * c';
        W(:, :, 4, 3) = -tl * c;
        W(:, :, 4, 4) = id;

        Hs{i} = W;
    end

    Hs{1} = Hs{1}(:, :, end, :); %첫번째 Hamiltonian chain 3번 leg dummy로
    Hs{end} = Hs{end}(:, :, :, 1); %마지막 Hamiltonian chain 4번 leg dummy로
end
```

Then set the parameters, and set the t list(hopping coefficient) for sub-problem a, b, and c.

```matlab
 % DMRG parameter
N_sweep = 5;
L = 40;
physical_dim = 2;
N_keep_list = [30, 40, 50, 60, 70];

l = 1:L-1;
t_a = ones(size(l));
t_b = 1.2.^(-(l-1));
t_c = 2 * rand(size(l)) - 1;
% 3 different hopping coefficient list
```

For sub-problem a, let's set the MPO.

```
MPO = tb_chain_MPO(L, t_a);
```

Now, a figure is plotted for the case of MPS by iterative diagonalization and 1 site update.

```matlab
figure;
hold on;
for i = 1 : 5
    N_keep = N_keep_list(i);
    fprintf('Nkeep value : %d', N_keep);
    [M, E_G1, E_list] = my_dmrg(MPO, N_keep, N_sweep, 0, 1, L, physical_dim); %MPS
by iterative diagonalization, 1 site update dmrg
    [E_G2,d_G,e_1p] = nonIntTB (-t_a);
    Error_list = abs(E_list(end, :)- E_G2);
    plot(1:N_sweep*2, Error_list, 'DisplayName', ['Nkeep :', num2str(N_keep)]);
end
```

```
Nkeep value : 30
25-05-20 14:05:55 | Sweep #1 of 10 (right -> left) : Energy = -25.10765
25-05-20 14:05:55 | Sweep #2 of 10 (left -> right) : Energy = -25.10779
25-05-20 14:05:55 | Sweep #3 of 10 (right -> left) : Energy = -25.10779
25-05-20 14:05:55 | Sweep #4 of 10 (left -> right) : Energy = -25.10779
25-05-20 14:05:55 | Sweep #5 of 10 (right -> left) : Energy = -25.10779
25-05-20 14:05:55 | Sweep #6 of 10 (left -> right) : Energy = -25.1078
25-05-20 14:05:56 | Sweep #7 of 10 (right -> left) : Energy = -25.1078
25-05-20 14:05:56 | Sweep #8 of 10 (left -> right) : Energy = -25.1078
25-05-20 14:05:56 | Sweep #9 of 10 (right -> left) : Energy = -25.1078
25-05-20 14:05:56 | Sweep #10 of 10 (left -> right) : Energy = -25.1078
Nkeep value : 40
25-05-20 14:05:56 | Sweep #1 of 10 (right -> left) : Energy = -25.10771
25-05-20 14:05:57 | Sweep #2 of 10 (left -> right) : Energy = -25.1078
25-05-20 14:05:57 | Sweep #3 of 10 (right -> left) : Energy = -25.1078
25-05-20 14:05:57 | Sweep #4 of 10 (left -> right) : Energy = -25.1078
25-05-20 14:05:57 | Sweep #5 of 10 (right -> left) : Energy = -25.1078
25-05-20 14:05:57 | Sweep #6 of 10 (left -> right) : Energy = -25.1078
25-05-20 14:05:57 | Sweep #7 of 10 (right -> left) : Energy = -25.1078
25-05-20 14:05:58 | Sweep #8 of 10 (left -> right) : Energy = -25.1078
25-05-20 14:05:58 | Sweep #9 of 10 (right -> left) : Energy = -25.1078
25-05-20 14:05:58 | Sweep #10 of 10 (left -> right) : Energy = -25.1078
Nkeep value : 50
25-05-20 14:05:58 | Sweep #1 of 10 (right -> left) : Energy = -25.10775
25-05-20 14:05:59 | Sweep #2 of 10 (left -> right) : Energy = -25.1078
25-05-20 14:05:59 | Sweep #3 of 10 (right -> left) : Energy = -25.1078
25-05-20 14:05:59 | Sweep #4 of 10 (left -> right) : Energy = -25.1078
25-05-20 14:05:59 | Sweep #5 of 10 (right -> left) : Energy = -25.1078
25-05-20 14:06:00 | Sweep #6 of 10 (left -> right) : Energy = -25.1078
25-05-20 14:06:00 | Sweep #7 of 10 (right -> left) : Energy = -25.1078
25-05-20 14:06:00 | Sweep #8 of 10 (left -> right) : Energy = -25.1078
25-05-20 14:06:00 | Sweep #9 of 10 (right -> left) : Energy = -25.1078
25-05-20 14:06:01 | Sweep #10 of 10 (left -> right) : Energy = -25.1078
Nkeep value : 60
25-05-20 14:06:01 | Sweep #1 of 10 (right -> left) : Energy = -25.10776
25-05-20 14:06:01 | Sweep #2 of 10 (left -> right) : Energy = -25.1078
25-05-20 14:06:02 | Sweep #3 of 10 (right -> left) : Energy = -25.1078
25-05-20 14:06:02 | Sweep #4 of 10 (left -> right) : Energy = -25.1078
25-05-20 14:06:02 | Sweep #5 of 10 (right -> left) : Energy = -25.1078
25-05-20 14:06:03 | Sweep #6 of 10 (left -> right) : Energy = -25.1078
25-05-20 14:06:03 | Sweep #7 of 10 (right -> left) : Energy = -25.1078
25-05-20 14:06:03 | Sweep #8 of 10 (left -> right) : Energy = -25.1078
```

```
25-05-20 14:06:03 | Sweep #9 of 10 (right -> left) : Energy = -25.1078
25-05-20 14:06:03 | Sweep #10 of 10 (left -> right) : Energy = -25.1078
Nkeep value : 70
25-05-20 14:06:04 | Sweep #1 of 10 (right -> left) : Energy = -25.10779
25-05-20 14:06:04 | Sweep #2 of 10 (left -> right) : Energy = -25.1078
25-05-20 14:06:05 | Sweep #3 of 10 (right -> left) : Energy = -25.1078
25-05-20 14:06:05 | Sweep #4 of 10 (left -> right) : Energy = -25.1078
25-05-20 14:06:05 | Sweep #5 of 10 (right -> left) : Energy = -25.1078
25-05-20 14:06:05 | Sweep #6 of 10 (left -> right) : Energy = -25.1078
25-05-20 14:06:06 | Sweep #7 of 10 (right -> left) : Energy = -25.1078
25-05-20 14:06:06 | Sweep #8 of 10 (left -> right) : Energy = -25.1078
25-05-20 14:06:07 | Sweep #9 of 10 (right -> left) : Energy = -25.1078
25-05-20 14:06:07 | Sweep #10 of 10 (left -> right) : Energy = -25.1078
```

```
fprintf('E_G_true = %.6g, d_G = %i\n',E_G2,d_G);
```
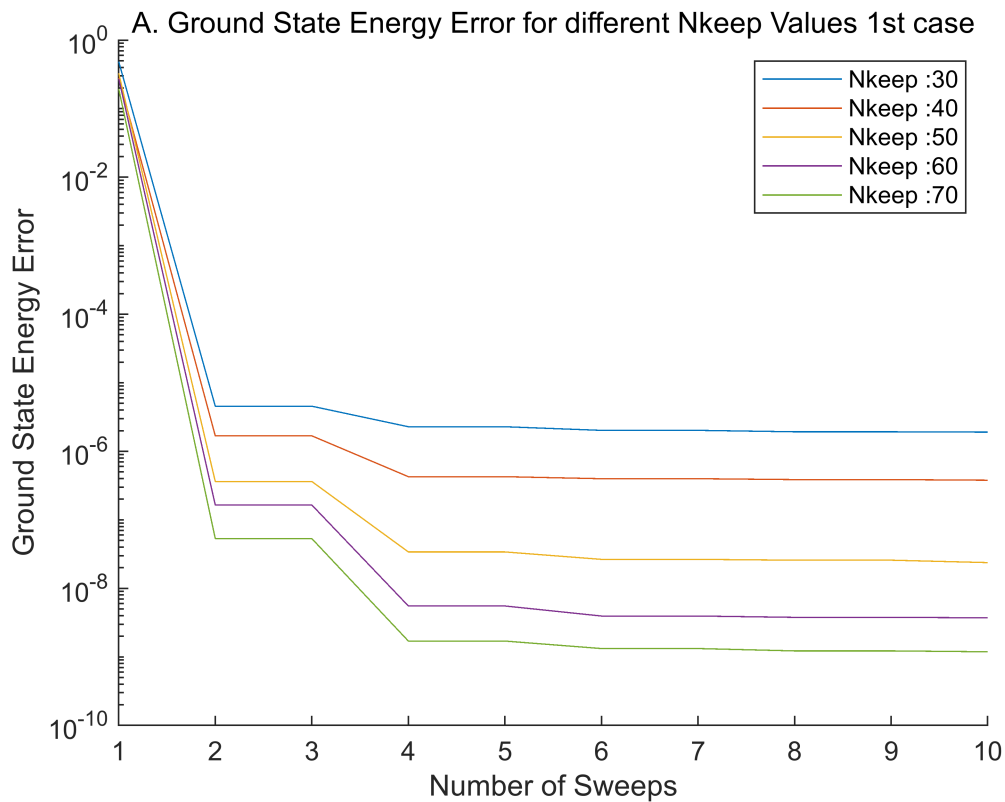
E_G_true = -25.1078, d_G = 1

```
hold off;
yscale('log');
legend show;

title('A. Ground State Energy Error for different Nkeep Values 1st case');
xlabel('Number of Sweeps');
ylabel('Ground State Energy Error');
```


Now for random MPS and 1 site update:

```matlab
figure;
hold on;
for i = 1 : 5
    N_keep = N_keep_list(i);
    fprintf('Nkeep value : %d', N_keep);
    [M, E_G1, E_list] = my_dmrg(MPO, N_keep, N_sweep, 1, 1, L, physical_dim);
%random generated MPS, 1 site update dmrg
    [E_G2,d_G,e_1p] = nonIntTB (-t_a);
    Error_list = abs(E_list(end, :)- E_G2);
    plot(1:N_sweep*2, Error_list, 'DisplayName', ['Nkeep :', num2str(N_keep)]);
end
```

```
Nkeep value : 30
25-05-20 14:06:27 | Sweep #1 of 10 (right -> left) : Energy = -23.39265
25-05-20 14:06:27 | Sweep #2 of 10 (left -> right) : Energy = -25.03686
25-05-20 14:06:27 | Sweep #3 of 10 (right -> left) : Energy = -25.10362
25-05-20 14:06:28 | Sweep #4 of 10 (left -> right) : Energy = -25.10766
25-05-20 14:06:28 | Sweep #5 of 10 (right -> left) : Energy = -25.10779
25-05-20 14:06:28 | Sweep #6 of 10 (left -> right) : Energy = -25.10779
25-05-20 14:06:28 | Sweep #7 of 10 (right -> left) : Energy = -25.1078
25-05-20 14:06:28 | Sweep #8 of 10 (left -> right) : Energy = -25.1078
25-05-20 14:06:28 | Sweep #9 of 10 (right -> left) : Energy = -25.1078
25-05-20 14:06:28 | Sweep #10 of 10 (left -> right) : Energy = -25.1078
Nkeep value : 40
25-05-20 14:06:29 | Sweep #1 of 10 (right -> left) : Energy = -23.62091
25-05-20 14:06:29 | Sweep #2 of 10 (left -> right) : Energy = -25.02481
25-05-20 14:06:29 | Sweep #3 of 10 (right -> left) : Energy = -25.09087
25-05-20 14:06:29 | Sweep #4 of 10 (left -> right) : Energy = -25.10643
25-05-20 14:06:29 | Sweep #5 of 10 (right -> left) : Energy = -25.10778
25-05-20 14:06:30 | Sweep #6 of 10 (left -> right) : Energy = -25.1078
25-05-20 14:06:30 | Sweep #7 of 10 (right -> left) : Energy = -25.1078
25-05-20 14:06:30 | Sweep #8 of 10 (left -> right) : Energy = -25.1078
25-05-20 14:06:30 | Sweep #9 of 10 (right -> left) : Energy = -25.1078
25-05-20 14:06:30 | Sweep #10 of 10 (left -> right) : Energy = -25.1078
Nkeep value : 50
25-05-20 14:06:31 | Sweep #1 of 10 (right -> left) : Energy = -23.86936
25-05-20 14:06:31 | Sweep #2 of 10 (left -> right) : Energy = -25.07601
25-05-20 14:06:31 | Sweep #3 of 10 (right -> left) : Energy = -25.10714
25-05-20 14:06:31 | Sweep #4 of 10 (left -> right) : Energy = -25.10779
25-05-20 14:06:32 | Sweep #5 of 10 (right -> left) : Energy = -25.1078
25-05-20 14:06:32 | Sweep #6 of 10 (left -> right) : Energy = -25.1078
25-05-20 14:06:32 | Sweep #7 of 10 (right -> left) : Energy = -25.1078
25-05-20 14:06:32 | Sweep #8 of 10 (left -> right) : Energy = -25.1078
25-05-20 14:06:33 | Sweep #9 of 10 (right -> left) : Energy = -25.1078
25-05-20 14:06:33 | Sweep #10 of 10 (left -> right) : Energy = -25.1078
Nkeep value : 60
25-05-20 14:06:33 | Sweep #1 of 10 (right -> left) : Energy = -23.44901
25-05-20 14:06:33 | Sweep #2 of 10 (left -> right) : Energy = -25.0461
25-05-20 14:06:34 | Sweep #3 of 10 (right -> left) : Energy = -25.10329
25-05-20 14:06:34 | Sweep #4 of 10 (left -> right) : Energy = -25.10775
25-05-20 14:06:34 | Sweep #5 of 10 (right -> left) : Energy = -25.1078
25-05-20 14:06:35 | Sweep #6 of 10 (left -> right) : Energy = -25.1078
25-05-20 14:06:35 | Sweep #7 of 10 (right -> left) : Energy = -25.1078
25-05-20 14:06:35 | Sweep #8 of 10 (left -> right) : Energy = -25.1078
25-05-20 14:06:35 | Sweep #9 of 10 (right -> left) : Energy = -25.1078
25-05-20 14:06:36 | Sweep #10 of 10 (left -> right) : Energy = -25.1078
Nkeep value : 70
25-05-20 14:06:36 | Sweep #1 of 10 (right -> left) : Energy = -23.44267
25-05-20 14:06:36 | Sweep #2 of 10 (left -> right) : Energy = -25.07666
25-05-20 14:06:37 | Sweep #3 of 10 (right -> left) : Energy = -25.10487
25-05-20 14:06:37 | Sweep #4 of 10 (left -> right) : Energy = -25.10771
```

```
25-05-20 14:06:38 | Sweep #5 of 10 (right -> left) : Energy = -25.1078
25-05-20 14:06:38 | Sweep #6 of 10 (left -> right) : Energy = -25.1078
25-05-20 14:06:39 | Sweep #7 of 10 (right -> left) : Energy = -25.1078
25-05-20 14:06:39 | Sweep #8 of 10 (left -> right) : Energy = -25.1078
25-05-20 14:06:39 | Sweep #9 of 10 (right -> left) : Energy = -25.1078
25-05-20 14:06:40 | Sweep #10 of 10 (left -> right) : Energy = -25.1078
```

```
fprintf('E_G_true = %.6g, d_G = %i\n',E_G2,d_G);
```
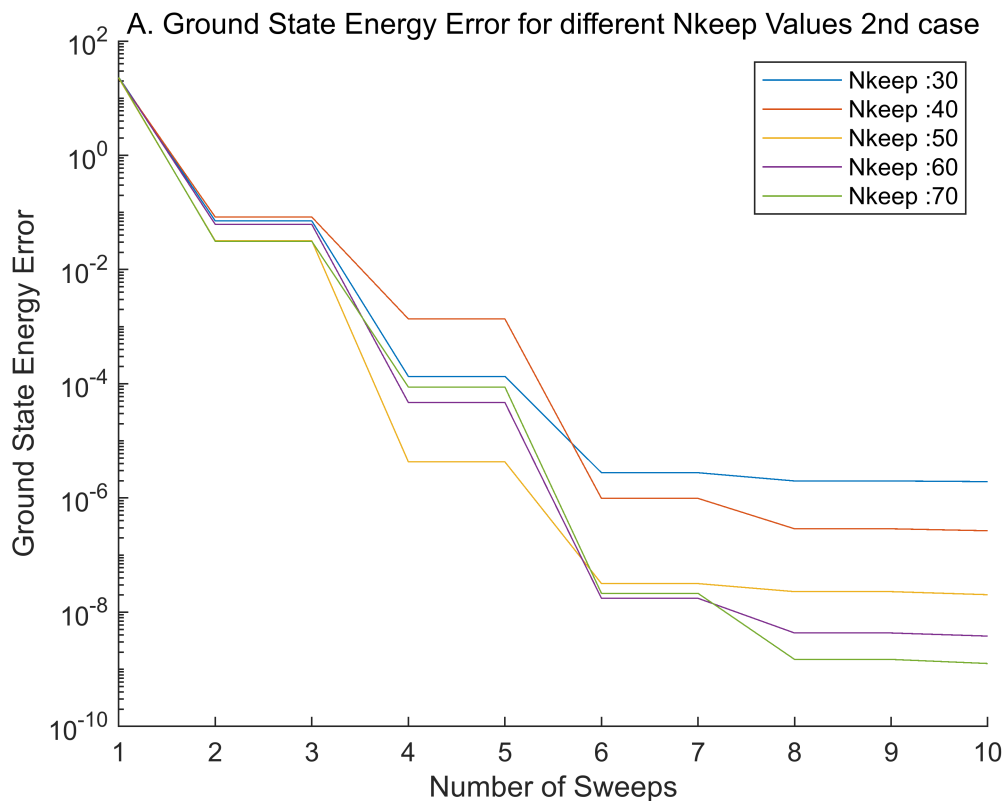
```
E_G_true = -25.1078, d_G = 1
```

```
hold off;
yscale('log');
legend show;

title('A. Ground State Energy Error for different Nkeep Values 2nd case');
xlabel('Number of Sweeps');
ylabel('Ground State Energy Error');
```


for MPS by iterative diagonalization and 2 site update:

```
figure;
hold on;
for i = 1 : 5
    N_keep = N_keep_list(i);
    fprintf('Nkeep value : %d', N_keep);
```

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```matlab
    [M, E_G1, E_list] = my_dmrg(MPO, N_keep, N_sweep, 0, 2, L, physical_dim); %MPS
by iterative diagonalization, 2 site update dmrg
    [E_G2,d_G,e_1p] = nonIntTB (-t_a);
    Error_list = abs(E_list(end, :)- E_G2);
    plot(1:N_sweep*2, Error_list, 'DisplayName', ['Nkeep :', num2str(N_keep)]);
end
```

```
Nkeep value : 30
25-05-20 14:06:54 | Sweep #1 of 10 (right -> left) : Energy = -25.10774
25-05-20 14:06:55 | Sweep #2 of 10 (left -> right) : Energy = -25.10779
25-05-20 14:06:55 | Sweep #3 of 10 (right -> left) : Energy = -25.1078
25-05-20 14:06:55 | Sweep #4 of 10 (left -> right) : Energy = -25.1078
25-05-20 14:06:55 | Sweep #5 of 10 (right -> left) : Energy = -25.1078
25-05-20 14:06:55 | Sweep #6 of 10 (left -> right) : Energy = -25.1078
25-05-20 14:06:56 | Sweep #7 of 10 (right -> left) : Energy = -25.1078
25-05-20 14:06:56 | Sweep #8 of 10 (left -> right) : Energy = -25.1078
25-05-20 14:06:56 | Sweep #9 of 10 (right -> left) : Energy = -25.1078
25-05-20 14:06:56 | Sweep #10 of 10 (left -> right) : Energy = -25.1078
Nkeep value : 40
25-05-20 14:06:57 | Sweep #1 of 10 (right -> left) : Energy = -25.10774
25-05-20 14:06:57 | Sweep #2 of 10 (left -> right) : Energy = -25.1078
25-05-20 14:06:57 | Sweep #3 of 10 (right -> left) : Energy = -25.1078
25-05-20 14:06:58 | Sweep #4 of 10 (left -> right) : Energy = -25.1078
25-05-20 14:06:58 | Sweep #5 of 10 (right -> left) : Energy = -25.1078
25-05-20 14:06:58 | Sweep #6 of 10 (left -> right) : Energy = -25.1078
25-05-20 14:06:59 | Sweep #7 of 10 (right -> left) : Energy = -25.1078
25-05-20 14:06:59 | Sweep #8 of 10 (left -> right) : Energy = -25.1078
25-05-20 14:06:59 | Sweep #9 of 10 (right -> left) : Energy = -25.1078
25-05-20 14:06:59 | Sweep #10 of 10 (left -> right) : Energy = -25.1078
Nkeep value : 50
25-05-20 14:07:00 | Sweep #1 of 10 (right -> left) : Energy = -25.10779
25-05-20 14:07:00 | Sweep #2 of 10 (left -> right) : Energy = -25.1078
25-05-20 14:07:01 | Sweep #3 of 10 (right -> left) : Energy = -25.1078
25-05-20 14:07:01 | Sweep #4 of 10 (left -> right) : Energy = -25.1078
25-05-20 14:07:01 | Sweep #5 of 10 (right -> left) : Energy = -25.1078
25-05-20 14:07:02 | Sweep #6 of 10 (left -> right) : Energy = -25.1078
25-05-20 14:07:02 | Sweep #7 of 10 (right -> left) : Energy = -25.1078
25-05-20 14:07:03 | Sweep #8 of 10 (left -> right) : Energy = -25.1078
25-05-20 14:07:03 | Sweep #9 of 10 (right -> left) : Energy = -25.1078
25-05-20 14:07:03 | Sweep #10 of 10 (left -> right) : Energy = -25.1078
Nkeep value : 60
25-05-20 14:07:04 | Sweep #1 of 10 (right -> left) : Energy = -25.10779
25-05-20 14:07:05 | Sweep #2 of 10 (left -> right) : Energy = -25.1078
25-05-20 14:07:05 | Sweep #3 of 10 (right -> left) : Energy = -25.1078
25-05-20 14:07:05 | Sweep #4 of 10 (left -> right) : Energy = -25.1078
25-05-20 14:07:06 | Sweep #5 of 10 (right -> left) : Energy = -25.1078
25-05-20 14:07:06 | Sweep #6 of 10 (left -> right) : Energy = -25.1078
25-05-20 14:07:06 | Sweep #7 of 10 (right -> left) : Energy = -25.1078
25-05-20 14:07:07 | Sweep #8 of 10 (left -> right) : Energy = -25.1078
25-05-20 14:07:07 | Sweep #9 of 10 (right -> left) : Energy = -25.1078
25-05-20 14:07:07 | Sweep #10 of 10 (left -> right) : Energy = -25.1078
Nkeep value : 70
25-05-20 14:07:08 | Sweep #1 of 10 (right -> left) : Energy = -25.10779
25-05-20 14:07:09 | Sweep #2 of 10 (left -> right) : Energy = -25.1078
25-05-20 14:07:09 | Sweep #3 of 10 (right -> left) : Energy = -25.1078
25-05-20 14:07:09 | Sweep #4 of 10 (left -> right) : Energy = -25.1078
25-05-20 14:07:10 | Sweep #5 of 10 (right -> left) : Energy = -25.1078
25-05-20 14:07:10 | Sweep #6 of 10 (left -> right) : Energy = -25.1078
25-05-20 14:07:11 | Sweep #7 of 10 (right -> left) : Energy = -25.1078
25-05-20 14:07:11 | Sweep #8 of 10 (left -> right) : Energy = -25.1078
25-05-20 14:07:12 | Sweep #9 of 10 (right -> left) : Energy = -25.1078
25-05-20 14:07:13 | Sweep #10 of 10 (left -> right) : Energy = -25.1078
```
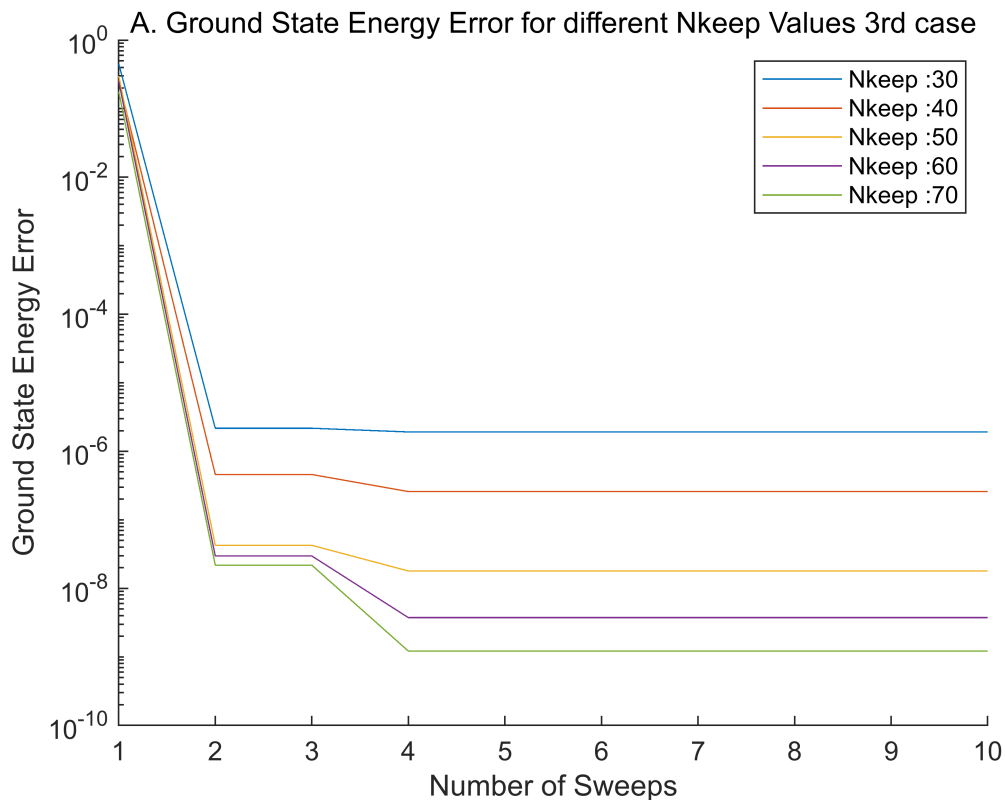
```
fprintf('E_G_true = %.6g, d_G = %i\n',E_G2,d_G);
```

E_G_true = -25.1078, d_G = 1

```
hold off;
yscale('log');
legend show;

title('A. Ground State Energy Error for different Nkeep Values 3rd case');
xlabel('Number of Sweeps');
ylabel('Ground State Energy Error');
```


A. Ground State Energy Error for different Nkeep Values 3rd case

Lastly, for random MPS and 2 site update:

```
figure;
hold on;
for i = 1 : 5
    N_keep = N_keep_list(i);
    fprintf('Nkeep value : %d', N_keep);
    [M, E_G1, E_list] = my_dmrg(MPO, N_keep, N_sweep, 1, 2, L, physical_dim);
%random MPS, 2 site update dmrg
    [E_G2,d_G,e_1p] = nonIntTB (-t_a);
    Error_list = abs(E_list(end, :)- E_G2);
    plot(1:N_sweep*2, Error_list, 'DisplayName', ['Nkeep :', num2str(N_keep)]);
end
```

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```
Nkeep value : 30
25-05-20 14:07:25 | Sweep #1 of 10 (right -> left) : Energy = -23.45252
25-05-20 14:07:25 | Sweep #2 of 10 (left -> right) : Energy = -25.02248
25-05-20 14:07:25 | Sweep #3 of 10 (right -> left) : Energy = -25.09735
25-05-20 14:07:25 | Sweep #4 of 10 (left -> right) : Energy = -25.10748
25-05-20 14:07:26 | Sweep #5 of 10 (right -> left) : Energy = -25.10779
25-05-20 14:07:26 | Sweep #6 of 10 (left -> right) : Energy = -25.1078
25-05-20 14:07:26 | Sweep #7 of 10 (right -> left) : Energy = -25.1078
25-05-20 14:07:26 | Sweep #8 of 10 (left -> right) : Energy = -25.1078
25-05-20 14:07:27 | Sweep #9 of 10 (right -> left) : Energy = -25.1078
25-05-20 14:07:27 | Sweep #10 of 10 (left -> right) : Energy = -25.1078
Nkeep value : 40
25-05-20 14:07:27 | Sweep #1 of 10 (right -> left) : Energy = -23.89525
25-05-20 14:07:27 | Sweep #2 of 10 (left -> right) : Energy = -25.08259
25-05-20 14:07:28 | Sweep #3 of 10 (right -> left) : Energy = -25.10726
25-05-20 14:07:28 | Sweep #4 of 10 (left -> right) : Energy = -25.10779
25-05-20 14:07:28 | Sweep #5 of 10 (right -> left) : Energy = -25.1078
25-05-20 14:07:29 | Sweep #6 of 10 (left -> right) : Energy = -25.1078
25-05-20 14:07:29 | Sweep #7 of 10 (right -> left) : Energy = -25.1078
25-05-20 14:07:29 | Sweep #8 of 10 (left -> right) : Energy = -25.1078
25-05-20 14:07:29 | Sweep #9 of 10 (right -> left) : Energy = -25.1078
25-05-20 14:07:30 | Sweep #10 of 10 (left -> right) : Energy = -25.1078
Nkeep value : 50
25-05-20 14:07:30 | Sweep #1 of 10 (right -> left) : Energy = -24.48219
25-05-20 14:07:30 | Sweep #2 of 10 (left -> right) : Energy = -25.04447
25-05-20 14:07:31 | Sweep #3 of 10 (right -> left) : Energy = -25.10536
25-05-20 14:07:31 | Sweep #4 of 10 (left -> right) : Energy = -25.10776
25-05-20 14:07:31 | Sweep #5 of 10 (right -> left) : Energy = -25.1078
25-05-20 14:07:32 | Sweep #6 of 10 (left -> right) : Energy = -25.1078
25-05-20 14:07:32 | Sweep #7 of 10 (right -> left) : Energy = -25.1078
25-05-20 14:07:32 | Sweep #8 of 10 (left -> right) : Energy = -25.1078
25-05-20 14:07:33 | Sweep #9 of 10 (right -> left) : Energy = -25.1078
25-05-20 14:07:33 | Sweep #10 of 10 (left -> right) : Energy = -25.1078
Nkeep value : 60
25-05-20 14:07:34 | Sweep #1 of 10 (right -> left) : Energy = -23.82095
25-05-20 14:07:35 | Sweep #2 of 10 (left -> right) : Energy = -25.06048
25-05-20 14:07:36 | Sweep #3 of 10 (right -> left) : Energy = -25.09903
25-05-20 14:07:36 | Sweep #4 of 10 (left -> right) : Energy = -25.10742
25-05-20 14:07:37 | Sweep #5 of 10 (right -> left) : Energy = -25.10779
25-05-20 14:07:37 | Sweep #6 of 10 (left -> right) : Energy = -25.1078
25-05-20 14:07:38 | Sweep #7 of 10 (right -> left) : Energy = -25.1078
25-05-20 14:07:39 | Sweep #8 of 10 (left -> right) : Energy = -25.1078
25-05-20 14:07:39 | Sweep #9 of 10 (right -> left) : Energy = -25.1078
25-05-20 14:07:40 | Sweep #10 of 10 (left -> right) : Energy = -25.1078
Nkeep value : 70
25-05-20 14:07:41 | Sweep #1 of 10 (right -> left) : Energy = -23.60216
25-05-20 14:07:42 | Sweep #2 of 10 (left -> right) : Energy = -25.0856
25-05-20 14:07:43 | Sweep #3 of 10 (right -> left) : Energy = -25.10656
25-05-20 14:07:44 | Sweep #4 of 10 (left -> right) : Energy = -25.10776
25-05-20 14:07:44 | Sweep #5 of 10 (right -> left) : Energy = -25.1078
25-05-20 14:07:45 | Sweep #6 of 10 (left -> right) : Energy = -25.1078
25-05-20 14:07:46 | Sweep #7 of 10 (right -> left) : Energy = -25.1078
25-05-20 14:07:47 | Sweep #8 of 10 (left -> right) : Energy = -25.1078
25-05-20 14:07:47 | Sweep #9 of 10 (right -> left) : Energy = -25.1078
25-05-20 14:07:48 | Sweep #10 of 10 (left -> right) : Energy = -25.1078
```

```
fprintf('E_G_true = %.6g, d_G = %i\n',E_G2,d_G);
```
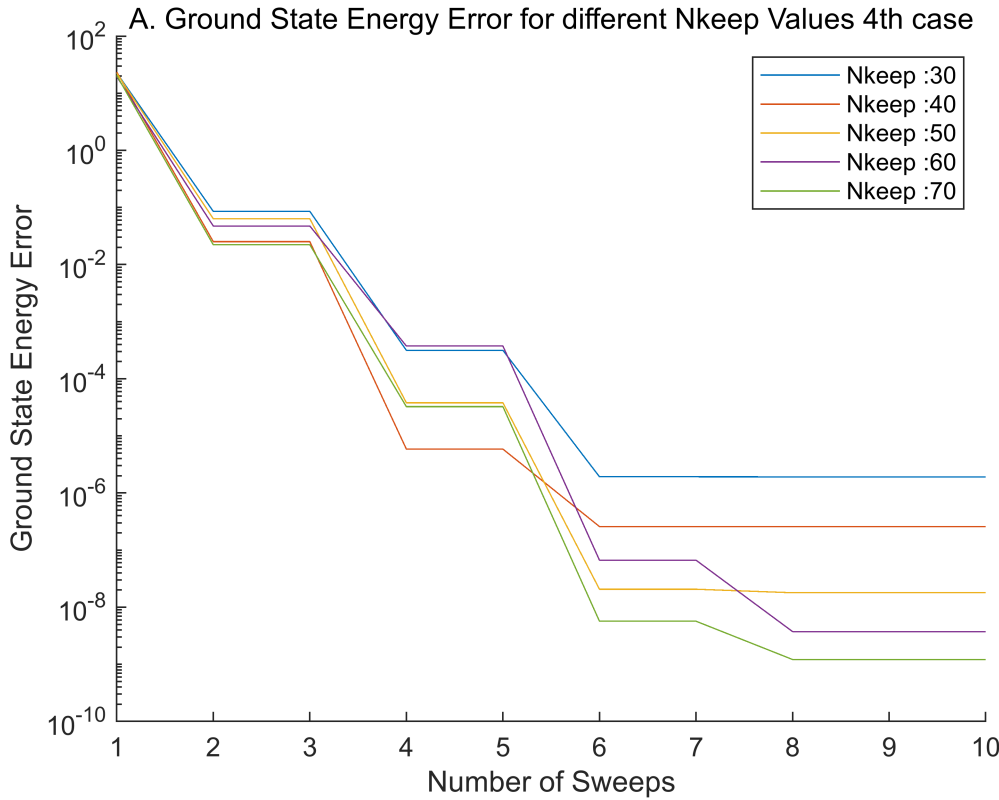
```
E_G_true = -25.1078, d_G = 1
```

```
hold off;
yscale('log');
```

```
legend show;

title('A. Ground State Energy Error for different Nkeep Values 4th case');
xlabel('Number of Sweeps');
ylabel('Ground State Energy Error');
```


A. Ground State Energy Error for different Nkeep Values 4th case

For the case of uniform hopping coefficients, only a few sweeps were required to reach the ground-state energy. As expected, a higher value of N_keep reduced the error overall. More sweeps were needed when using a random MPS compared to an MPS generated via iterative diagonalization. There was no significant difference observed between the single-site and two-site update methods.

Now, sub-problem b: use t_b for t list and repeat!

I suppressed the results obtained during the process from now on.

```
MPO = tb_chain_MPO(L, t_b);

fprintf('Sub-problem b, 1st case:')
```

Sub-problem b, 1st case:

```
figure;
hold on;
for i = 1 : 5
    N_keep = N_keep_list(i);
    [~, M, E_G1, E_list] = evalc('my_dmrg(MPO, N_keep, N_sweep, 0, 1, L,
physical_dim)'); %MPS by iterative diagonalization, 1 site update dmrg
```
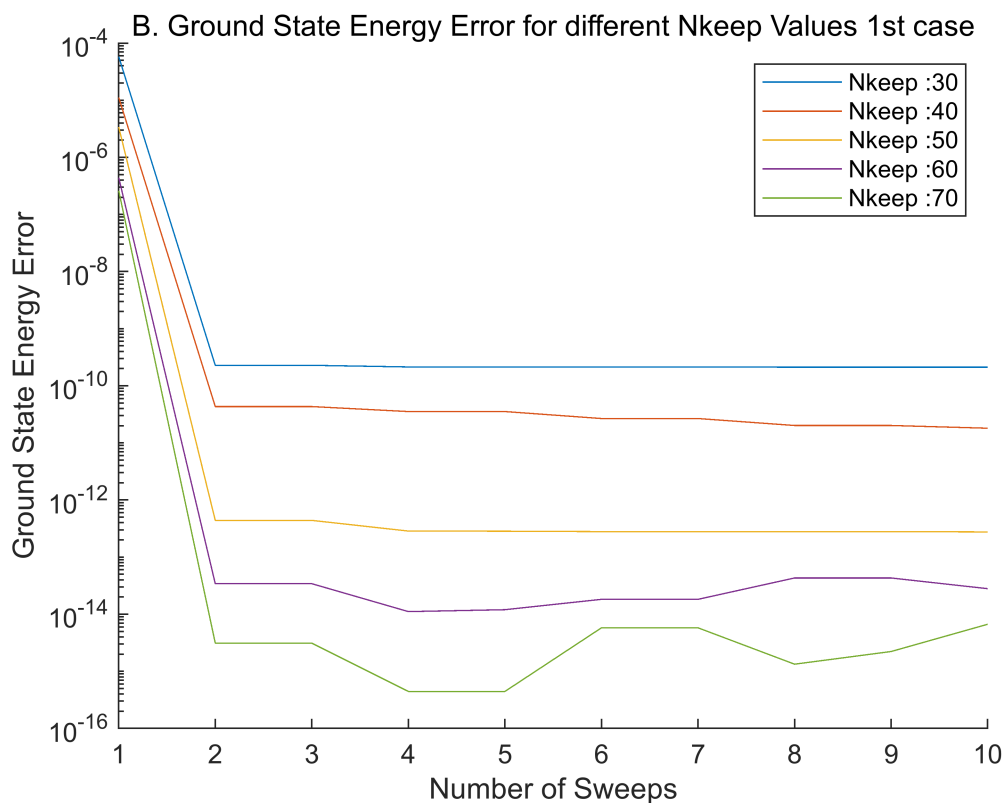
9

```matlab
    [E_G2,d_G,e_1p] = nonIntTB (-t_b);
    Error_list = abs(E_list(end, :)- E_G2);
    plot(1:N_sweep*2, Error_list, 'DisplayName', ['Nkeep :', num2str(N_keep)]);
end

hold off;
yscale('log');
legend show;

title('B. Ground State Energy Error for different Nkeep Values 1st case');
xlabel('Number of Sweeps');
ylabel('Ground State Energy Error');
```


B. Ground State Energy Error for different Nkeep Values 1st case

```matlab
fprintf('Sub-problem b, 2nd case:')
```
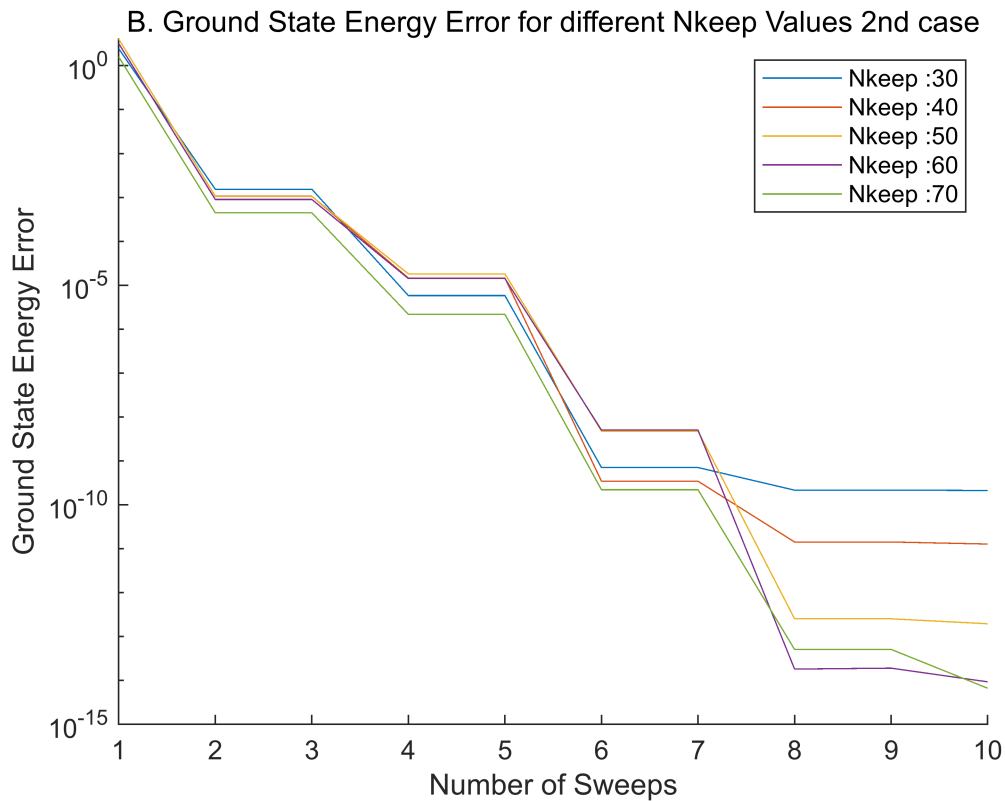
Sub-problem b, 2nd case:

```matlab
figure;
hold on;
for i = 1 : 5
    N_keep = N_keep_list(i);
    [~, M, E_G1, E_list] = evalc('my_dmrg(MPO, N_keep, N_sweep, 1, 1, L,
physical_dim)'); %random generated MPS, 1 site update dmrg
    [E_G2,d_G,e_1p] = nonIntTB (-t_b);
    Error_list = abs(E_list(end, :)- E_G2);
    plot(1:N_sweep*2, Error_list, 'DisplayName', ['Nkeep :', num2str(N_keep)]);
```

```
end

hold off;
yscale('log');
legend show;

title('B. Ground State Energy Error for different Nkeep Values 2nd case');
xlabel('Number of Sweeps');
ylabel('Ground State Energy Error');
```


B. Ground State Energy Error for different Nkeep Values 2nd case

```
fprintf('Sub-problem b, 3rd case:')
```
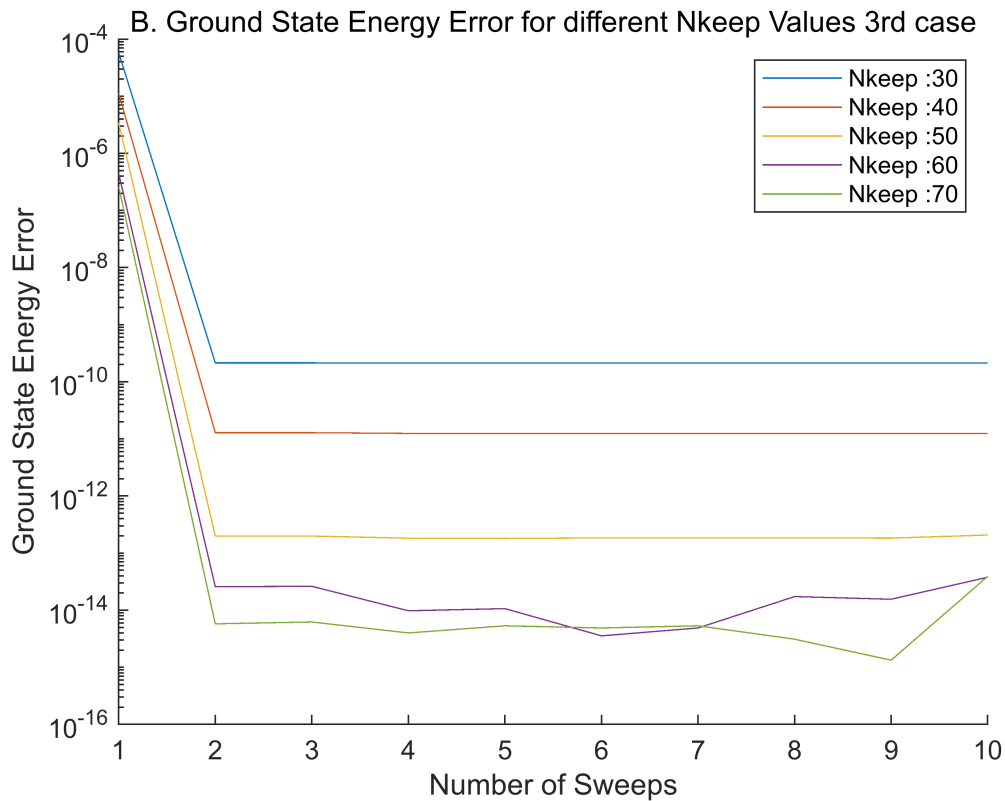
Sub-problem b, 3rd case:

```
figure;
hold on;
for i = 1 : 5
    N_keep = N_keep_list(i);
    [~, M, E_G1, E_list] = evalc('my_dmrg(MPO, N_keep, N_sweep, 0, 2, L,
physical_dim)'); %MPS by iterative diagonalization, 2 site update dmrg
    [E_G2,d_G,e_1p] = nonIntTB (-t_b);
    Error_list = abs(E_list(end, :)- E_G2);
    plot(1:N_sweep*2, Error_list, 'DisplayName', ['Nkeep :', num2str(N_keep)]);
end
```

```
hold off;
yscale('log');
legend show;

title('B. Ground State Energy Error for different Nkeep Values 3rd case');
xlabel('Number of Sweeps');
ylabel('Ground State Energy Error');
```


B. Ground State Energy Error for different Nkeep Values 3rd case

```
fprintf('Sub-problem b, 4th case:')
```
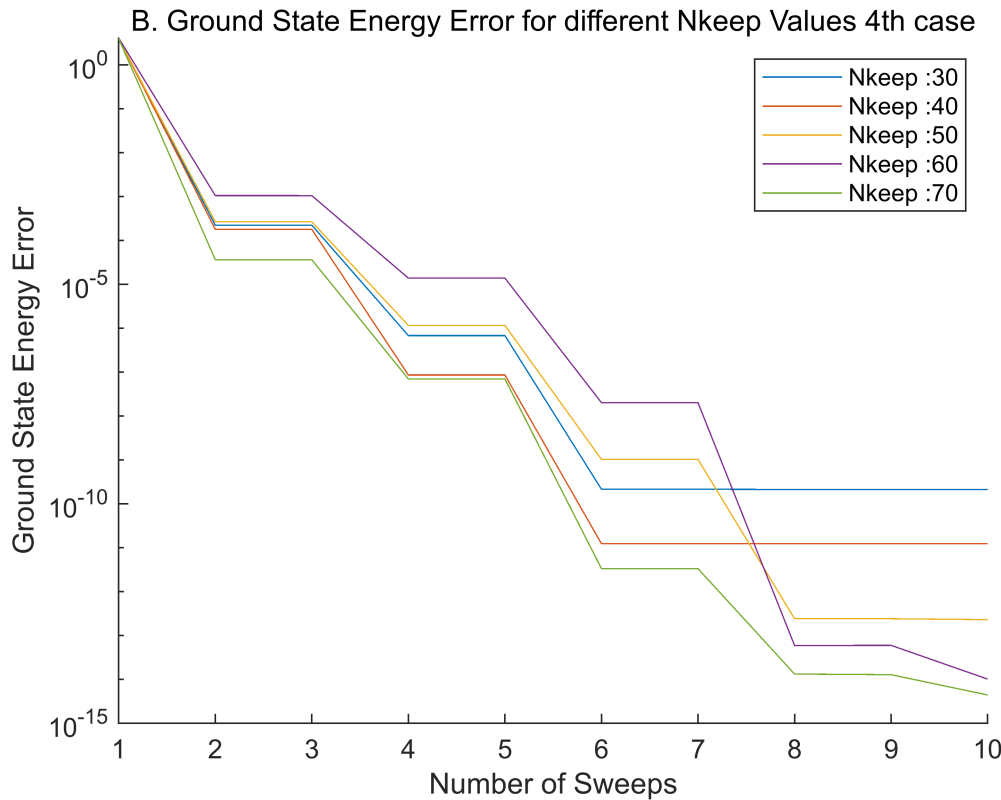
Sub-problem b, 4th case:

```
figure;
hold on;
for i = 1 : 5
    N_keep = N_keep_list(i);
    [~, M, E_G1, E_list] = evalc('my_dmrg(MPO, N_keep, N_sweep, 1, 2, L,
physical_dim)'); %random MPS, 2 site update dmrg
    [E_G2,d_G,e_1p] = nonIntTB (-t_b);
    Error_list = abs(E_list(end, :)- E_G2);
    plot(1:N_sweep*2, Error_list, 'DisplayName', ['Nkeep :', num2str(N_keep)]);
end


hold off;
yscale('log');
```

```
legend show;

title('B. Ground State Energy Error for different Nkeep Values 4th case');
xlabel('Number of Sweeps');
ylabel('Ground State Energy Error');
```


B. Ground State Energy Error for different Nkeep Values 4th case

In sub-problem (b), overall errors were lower compared to the uniform case. Due to the already low error, a slight increase in error was observed over the course of sweeps at higher N_keep values, but these variations were negligible. Other results were consistent with the observations from sub-problem (a).

For sub-problem c , do it again!

```
MPO = tb_chain_MPO(L, t_c);
fprintf('Sub-problem c, 1st case:')
```
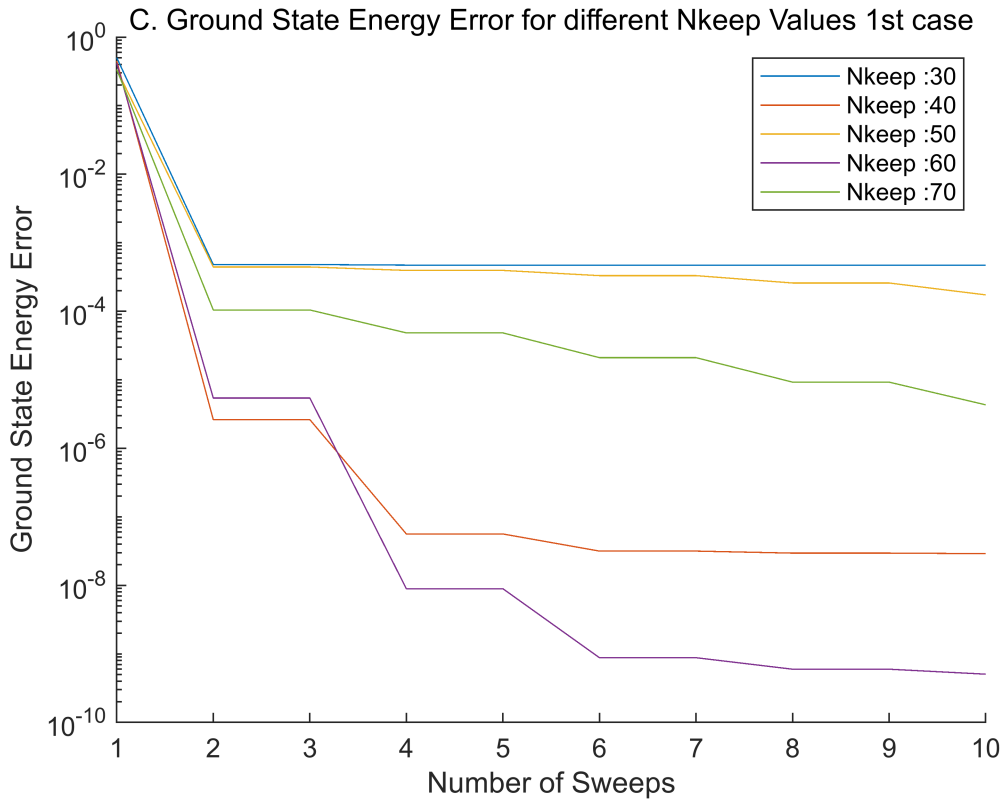
```
Sub-problem c, 1st case:
```

```
figure;
hold on;
for i = 1 : 5
    N_keep = N_keep_list(i);
    [~, M, E_G1, E_list] = evalc('my_dmrg(MPO, N_keep, N_sweep, 0, 1, L,
physical_dim)'); %MPS by iterative diagonalization, 1 site update dmrg
    [E_G2,d_G,e_1p] = nonIntTB (-t_c);
    Error_list = abs(E_list(end, :)- E_G2);
    plot(1:N_sweep*2, Error_list, 'DisplayName', ['Nkeep :', num2str(N_keep)]);
```

```
end

hold off;
yscale('log');
legend show;

title('C. Ground State Energy Error for different Nkeep Values 1st case');
xlabel('Number of Sweeps');
ylabel('Ground State Energy Error');
```


C. Ground State Energy Error for different Nkeep Values 1st case

```
fprintf('Sub-problem c, 2nd case:')
```
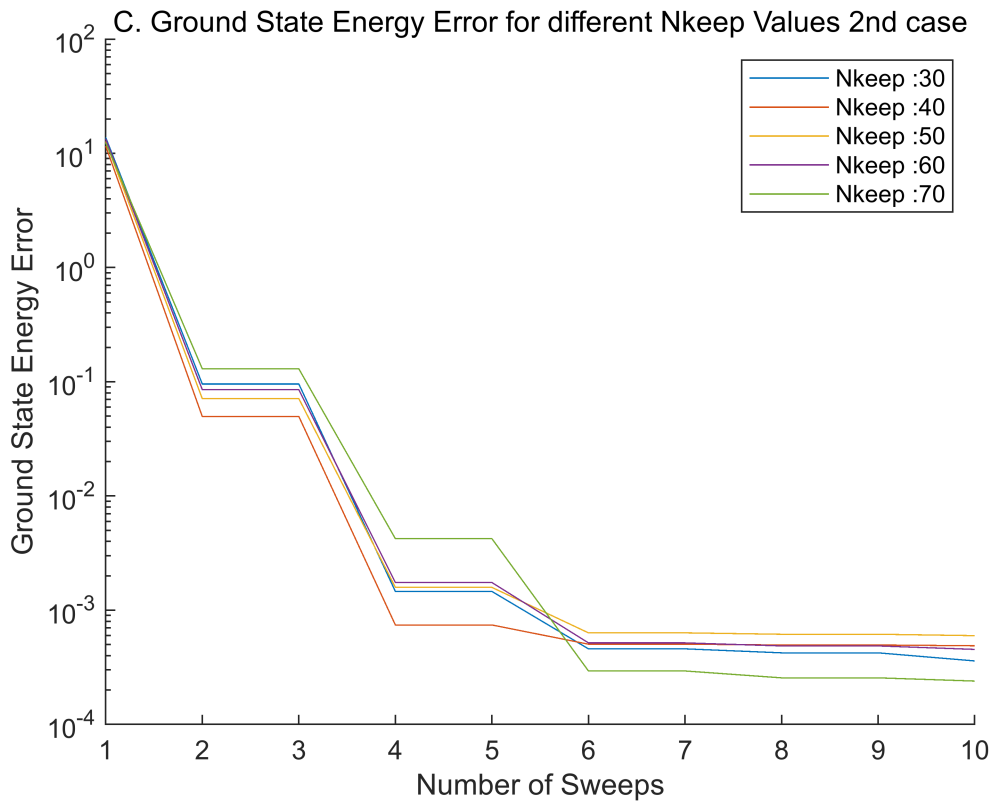
Sub-problem c, 2nd case:

```
figure;
hold on;
for i = 1 : 5
    N_keep = N_keep_list(i);
    [~, M, E_G1, E_list] = evalc('my_dmrg(MPO, N_keep, N_sweep, 1, 1, L,
physical_dim)'); %random generated MPS, 1 site update dmrg
    [E_G2,d_G,e_1p] = nonIntTB (-t_c);
    Error_list = abs(E_list(end, :)- E_G2);
    plot(1:N_sweep*2, Error_list, 'DisplayName', ['Nkeep :', num2str(N_keep)]);
end
```

```
hold off;
yscale('log');
legend show;

title('C. Ground State Energy Error for different Nkeep Values 2nd case');
xlabel('Number of Sweeps');
ylabel('Ground State Energy Error');
```


C. Ground State Energy Error for different Nkeep Values 2nd case

```
fprintf('Sub-problem c, 3rd case:')
```

Sub-problem c, 3rd case:

```
figure;
hold on;
for i = 1 : 5
    N_keep = N_keep_list(i);
    [~, M, E_G1, E_list] = evalc('my_dmrg(MPO, N_keep, N_sweep, 0, 2, L,
physical_dim)'); %MPS by iterative diagonalization, 2 site update dmrg
    [E_G2,d_G,e_1p] = nonIntTB (-t_c);
    Error_list = abs(E_list(end, :)- E_G2);
    plot(1:N_sweep*2, Error_list, 'DisplayName', ['Nkeep :', num2str(N_keep)]);
end

hold off;
yscale('log');
legend show;
```
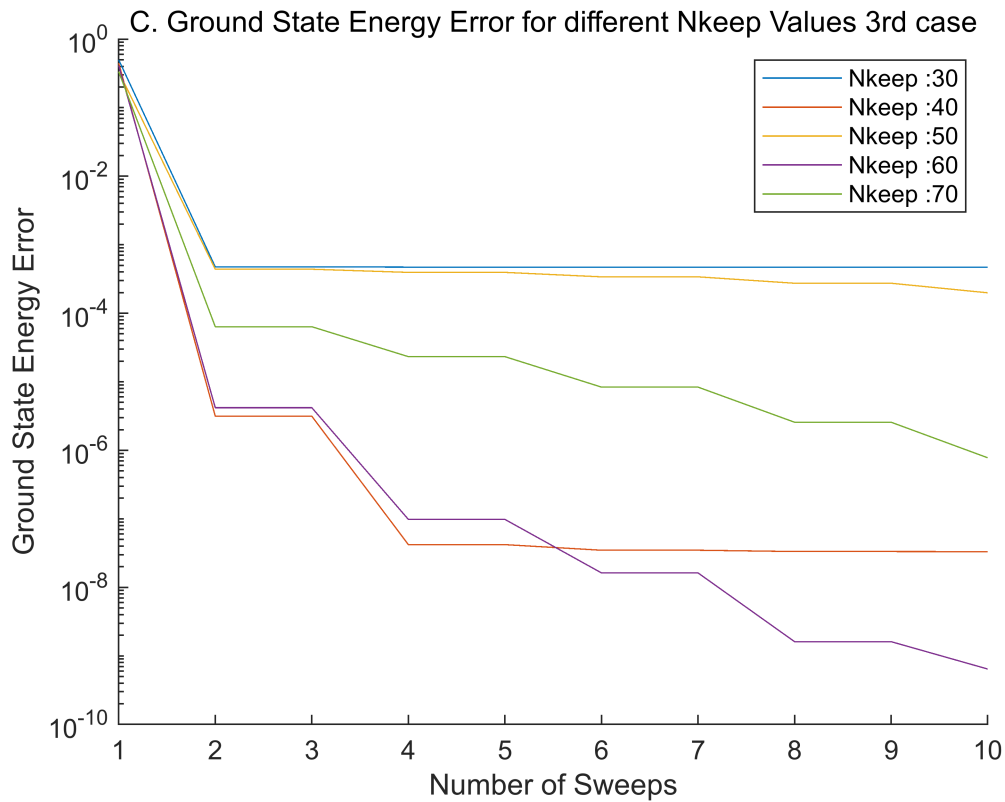
```
title('C. Ground State Energy Error for different Nkeep Values 3rd case');
xlabel('Number of Sweeps');
ylabel('Ground State Energy Error');
```


C. Ground State Energy Error for different Nkeep Values 3rd case

```
fprintf('Sub-problem c, 4th case:')
```

Sub-problem c, 4th case:

```
figure;
hold on;
for i = 1 : 5
    N_keep = N_keep_list(i);
    [~, M, E_G1, E_list] = evalc('my_dmrg(MPO, N_keep, N_sweep, 1, 2, L,
physical_dim)'); %random MPS, 2 site update dmrg
    [E_G2,d_G,e_1p] = nonIntTB (-t_c);
    Error_list = abs(E_list(end, :)- E_G2);
    plot(1:N_sweep*2, Error_list, 'DisplayName', ['Nkeep :', num2str(N_keep)]);
end


hold off;
yscale('log');
legend show;

title('C. Ground State Energy Error for different Nkeep Values 4th case');
```
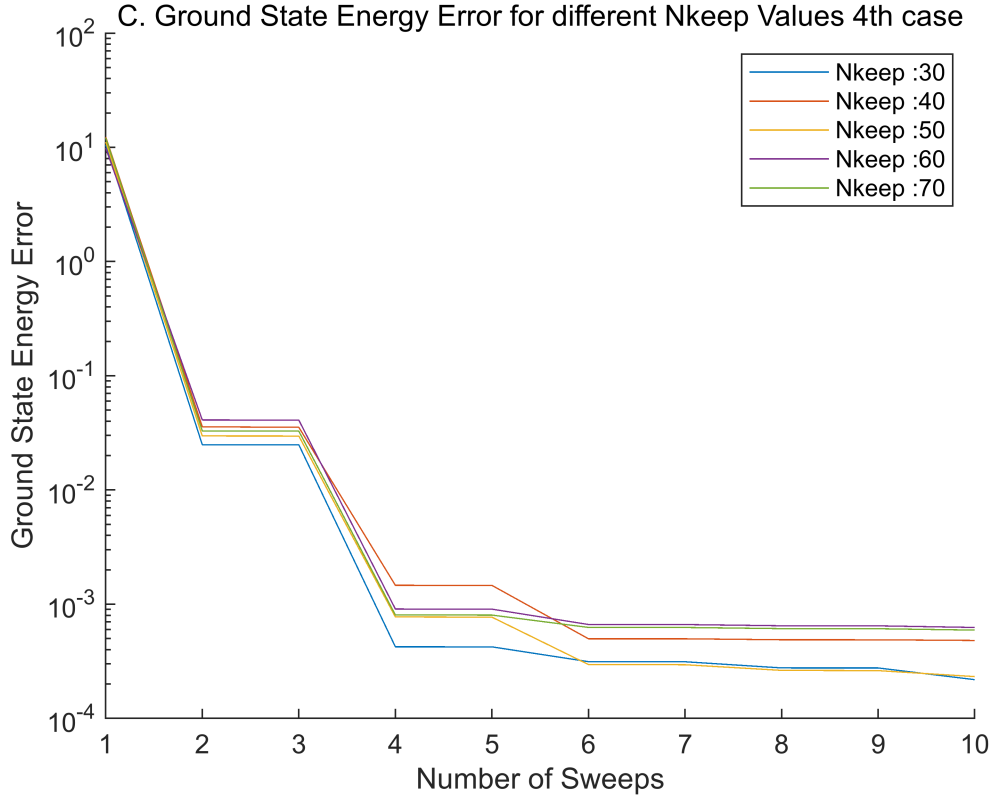
```
xlabel('Number of Sweeps');
ylabel('Ground State Energy Error');
```


C. Ground State Energy Error for different Nkeep Values 4th case

In sub-problem (c), the errors varied the most among the three cases. For random MPS, the error decreased only up to a certain point and did not improve further even as N_keep increased. In contrast, for MPS generated via iterative diagonalization, the error significantly decreased with higher N_keep values. Again, no notable difference was observed between the single-site and two-site update methods.

Problem 4. 1D Hubbard model

First, construct MPO.

```matlab
function Hs = Hubbard_MPO(L, U, t)
    c0 = [0,1,0,0; 0,0,0,0; 0,0,0,-1; 0,0,0,0];     % up-spin annihilation operator
    c1 = [0,0,1,0; 0,0,0,1; 0,0,0,0; 0,0,0,0];     % down-spin annihilation operator
    n0 = diag([0,1,0,1]);
    n1 = diag([0,0,1,1]);
    z = diag([1,-1,-1,1]);
    id = eye(4);

    Hs = cell(1,L);

    for i = 1:L
        W = zeros(4,4,6,6);

        W(:, :, 1, 1) = id;
        W(:, :, 2, 1) = c0' * z;
        W(:, :, 3, 1) = c1' * z;
        W(:, :, 4, 1) = z * c0;
        W(:, :, 5, 1) = z * c1;
        W(:, :, 6, 1) = 0.5 * U * (2*n0*n1 -n0-n1+id);
        W(:, :, 6, 2) = t*c0;
        W(:, :, 6, 3) = t*c1;
        W(:, :, 6, 4) = t*c0';
        W(:, :, 6, 5) = t*c1';
        W(:, :, 6, 6) = id;

        Hs{i} = W;
    end

    Hs{1} = Hs{1}(:, :, end, :); %첫번째 Hamiltonian chain 3번 leg dummy로
    Hs{end} = Hs{end}(:, :, :, 1); %마지막 Hamiltonian chain 4번 leg dummy로
end
```

Then, set the parameters and the list of N_keep.

```matlab
N_sweep = 5;
L = 40;
physical_dim = 4;
t = 1;
N_keep_list = 20:20:400;
```

Now, obtain the ground-state energy using DMRG(I implemented MPS by iterative diagonalization and 1 site update) for various values of N_keep. Furthermore, keep increasing N_keep until ground-state energy change is negligible.

```matlab
U = 2;
MPO = Hubbard_MPO(L, U, t);
```

```matlab
E_G_list = zeros(length(N_keep_list));
threshold = 1e-6;

figure;
for i = 1 : length(N_keep_list)
    N_keep = N_keep_list(i);
    [M, E_G, E_list] = my_dmrg(MPO, N_keep, N_sweep, 0, 1, L, physical_dim);
    E_G_list(i) = E_G;
    fprintf('Nkeep value : %d, E0 : %d', N_keep, E_G);
    if i>1 && abs((E_G - E_G_prev)/E_G_prev) < threshold
        last_idx = i;
        break;
    end
    E_G_prev = E_G;
end
```

```
25-05-20 15:31:42 | Sweep #1 of 10 (right -> left) : Energy = -32.8091
25-05-20 15:31:42 | Sweep #2 of 10 (left -> right) : Energy = -32.88891
25-05-20 15:31:42 | Sweep #3 of 10 (right -> left) : Energy = -32.93687
25-05-20 15:31:42 | Sweep #4 of 10 (left -> right) : Energy = -32.99099
25-05-20 15:31:42 | Sweep #5 of 10 (right -> left) : Energy = -33.03199
25-05-20 15:31:42 | Sweep #6 of 10 (left -> right) : Energy = -33.05888
25-05-20 15:31:43 | Sweep #7 of 10 (right -> left) : Energy = -33.08131
25-05-20 15:31:43 | Sweep #8 of 10 (left -> right) : Energy = -33.1018
25-05-20 15:31:43 | Sweep #9 of 10 (right -> left) : Energy = -33.12161
25-05-20 15:31:43 | Sweep #10 of 10 (left -> right) : Energy = -33.13661
Nkeep value : 20, E0 : -3.313661e+01
25-05-20 15:31:44 | Sweep #1 of 10 (right -> left) : Energy = -33.18828
25-05-20 15:31:44 | Sweep #2 of 10 (left -> right) : Energy = -33.20728
25-05-20 15:31:44 | Sweep #3 of 10 (right -> left) : Energy = -33.20917
25-05-20 15:31:44 | Sweep #4 of 10 (left -> right) : Energy = -33.21008
25-05-20 15:31:45 | Sweep #5 of 10 (right -> left) : Energy = -33.21061
25-05-20 15:31:45 | Sweep #6 of 10 (left -> right) : Energy = -33.21106
25-05-20 15:31:45 | Sweep #7 of 10 (right -> left) : Energy = -33.21139
25-05-20 15:31:45 | Sweep #8 of 10 (left -> right) : Energy = -33.21156
25-05-20 15:31:46 | Sweep #9 of 10 (right -> left) : Energy = -33.21164
25-05-20 15:31:46 | Sweep #10 of 10 (left -> right) : Energy = -33.21168
Nkeep value : 40, E0 : -3.321168e+01
25-05-20 15:31:47 | Sweep #1 of 10 (right -> left) : Energy = -33.20599
25-05-20 15:31:47 | Sweep #2 of 10 (left -> right) : Energy = -33.21837
25-05-20 15:31:48 | Sweep #3 of 10 (right -> left) : Energy = -33.21877
25-05-20 15:31:48 | Sweep #4 of 10 (left -> right) : Energy = -33.21892
25-05-20 15:31:49 | Sweep #5 of 10 (right -> left) : Energy = -33.2191
25-05-20 15:31:49 | Sweep #6 of 10 (left -> right) : Energy = -33.21922
25-05-20 15:31:49 | Sweep #7 of 10 (right -> left) : Energy = -33.21938
25-05-20 15:31:50 | Sweep #8 of 10 (left -> right) : Energy = -33.21951
25-05-20 15:31:50 | Sweep #9 of 10 (right -> left) : Energy = -33.21964
25-05-20 15:31:51 | Sweep #10 of 10 (left -> right) : Energy = -33.21987
Nkeep value : 60, E0 : -3.321987e+01
25-05-20 15:31:53 | Sweep #1 of 10 (right -> left) : Energy = -33.20958
25-05-20 15:31:53 | Sweep #2 of 10 (left -> right) : Energy = -33.21977
25-05-20 15:31:54 | Sweep #3 of 10 (right -> left) : Energy = -33.22105
25-05-20 15:31:55 | Sweep #4 of 10 (left -> right) : Energy = -33.22218
25-05-20 15:31:56 | Sweep #5 of 10 (right -> left) : Energy = -33.22238
25-05-20 15:31:57 | Sweep #6 of 10 (left -> right) : Energy = -33.22244
25-05-20 15:31:58 | Sweep #7 of 10 (right -> left) : Energy = -33.2225
25-05-20 15:31:59 | Sweep #8 of 10 (left -> right) : Energy = -33.22259
25-05-20 15:32:00 | Sweep #9 of 10 (right -> left) : Energy = -33.22268
25-05-20 15:32:02 | Sweep #10 of 10 (left -> right) : Energy = -33.22275
Nkeep value : 80, E0 : -3.322275e+01
```

```
25-05-20 15:32:05 | Sweep #1 of 10 (right -> left) : Energy = -33.21078
25-05-20 15:32:06 | Sweep #2 of 10 (left -> right) : Energy = -33.22203
25-05-20 15:32:08 | Sweep #3 of 10 (right -> left) : Energy = -33.22285
25-05-20 15:32:09 | Sweep #4 of 10 (left -> right) : Energy = -33.22335
25-05-20 15:32:11 | Sweep #5 of 10 (right -> left) : Energy = -33.22352
25-05-20 15:32:12 | Sweep #6 of 10 (left -> right) : Energy = -33.22357
25-05-20 15:32:14 | Sweep #7 of 10 (right -> left) : Energy = -33.2236
25-05-20 15:32:15 | Sweep #8 of 10 (left -> right) : Energy = -33.22362
25-05-20 15:32:17 | Sweep #9 of 10 (right -> left) : Energy = -33.22363
25-05-20 15:32:19 | Sweep #10 of 10 (left -> right) : Energy = -33.22364
Nkeep value : 100, E0 : -3.322364e+01
25-05-20 15:32:24 | Sweep #1 of 10 (right -> left) : Energy = -33.21636
25-05-20 15:32:26 | Sweep #2 of 10 (left -> right) : Energy = -33.22315
25-05-20 15:32:29 | Sweep #3 of 10 (right -> left) : Energy = -33.22374
25-05-20 15:32:33 | Sweep #4 of 10 (left -> right) : Energy = -33.22383
25-05-20 15:32:36 | Sweep #5 of 10 (right -> left) : Energy = -33.22385
25-05-20 15:32:40 | Sweep #6 of 10 (left -> right) : Energy = -33.22385
25-05-20 15:32:43 | Sweep #7 of 10 (right -> left) : Energy = -33.22386
25-05-20 15:32:46 | Sweep #8 of 10 (left -> right) : Energy = -33.22386
25-05-20 15:32:50 | Sweep #9 of 10 (right -> left) : Energy = -33.22386
25-05-20 15:32:53 | Sweep #10 of 10 (left -> right) : Energy = -33.22386
Nkeep value : 120, E0 : -3.322386e+01
25-05-20 15:33:03 | Sweep #1 of 10 (right -> left) : Energy = -33.21754
25-05-20 15:33:07 | Sweep #2 of 10 (left -> right) : Energy = -33.22293
25-05-20 15:33:11 | Sweep #3 of 10 (right -> left) : Energy = -33.22365
25-05-20 15:33:14 | Sweep #4 of 10 (left -> right) : Energy = -33.22389
25-05-20 15:33:18 | Sweep #5 of 10 (right -> left) : Energy = -33.22392
25-05-20 15:33:22 | Sweep #6 of 10 (left -> right) : Energy = -33.22393
25-05-20 15:33:26 | Sweep #7 of 10 (right -> left) : Energy = -33.22393
25-05-20 15:33:29 | Sweep #8 of 10 (left -> right) : Energy = -33.22393
25-05-20 15:33:32 | Sweep #9 of 10 (right -> left) : Energy = -33.22393
25-05-20 15:33:37 | Sweep #10 of 10 (left -> right) : Energy = -33.22394
Nkeep value : 140, E0 : -3.322394e+01
25-05-20 15:33:50 | Sweep #1 of 10 (right -> left) : Energy = -33.21859
25-05-20 15:33:54 | Sweep #2 of 10 (left -> right) : Energy = -33.22337
25-05-20 15:34:00 | Sweep #3 of 10 (right -> left) : Energy = -33.22393
25-05-20 15:34:03 | Sweep #4 of 10 (left -> right) : Energy = -33.22397
25-05-20 15:34:06 | Sweep #5 of 10 (right -> left) : Energy = -33.22398
25-05-20 15:34:11 | Sweep #6 of 10 (left -> right) : Energy = -33.22398
25-05-20 15:34:15 | Sweep #7 of 10 (right -> left) : Energy = -33.22398
25-05-20 15:34:19 | Sweep #8 of 10 (left -> right) : Energy = -33.22398
25-05-20 15:34:24 | Sweep #9 of 10 (right -> left) : Energy = -33.22399
25-05-20 15:34:28 | Sweep #10 of 10 (left -> right) : Energy = -33.22399
Nkeep value : 160, E0 : -3.322399e+01
25-05-20 15:34:40 | Sweep #1 of 10 (right -> left) : Energy = -33.21951
25-05-20 15:34:45 | Sweep #2 of 10 (left -> right) : Energy = -33.22366
25-05-20 15:34:52 | Sweep #3 of 10 (right -> left) : Energy = -33.22398
25-05-20 15:34:59 | Sweep #4 of 10 (left -> right) : Energy = -33.224
25-05-20 15:35:05 | Sweep #5 of 10 (right -> left) : Energy = -33.224
25-05-20 15:35:12 | Sweep #6 of 10 (left -> right) : Energy = -33.22401
25-05-20 15:35:19 | Sweep #7 of 10 (right -> left) : Energy = -33.22401
25-05-20 15:35:26 | Sweep #8 of 10 (left -> right) : Energy = -33.22401
25-05-20 15:35:32 | Sweep #9 of 10 (right -> left) : Energy = -33.22401
25-05-20 15:35:38 | Sweep #10 of 10 (left -> right) : Energy = -33.22401
Nkeep value : 180, E0 : -3.322401e+01
```
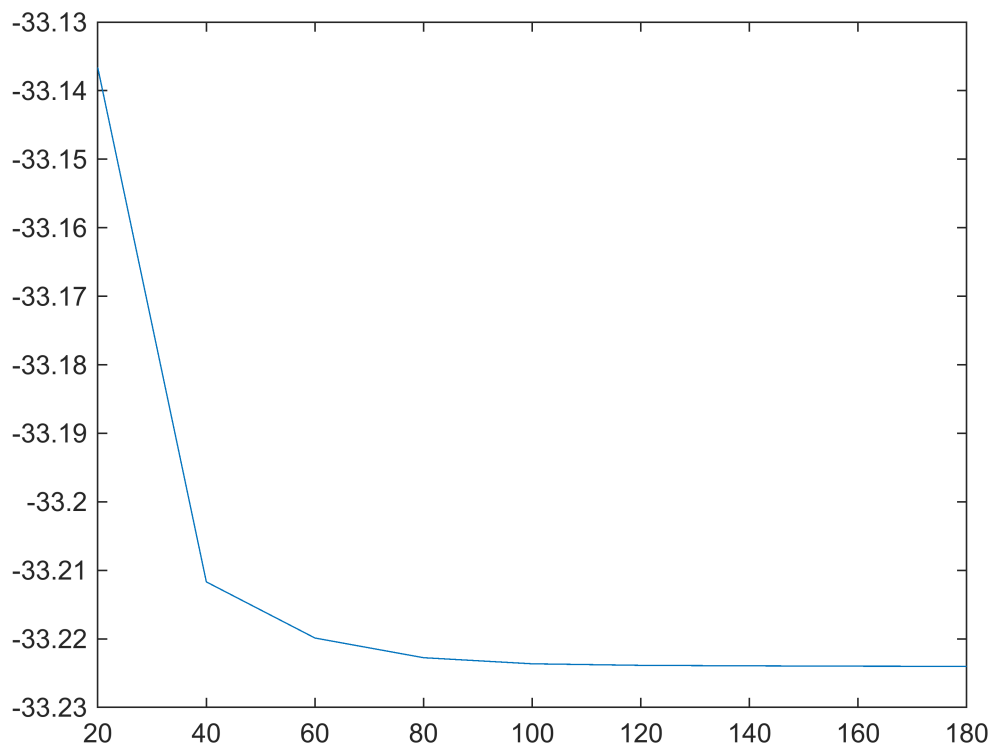
```
plot_list = E_G_list(1:last_idx);
plot_N_keep = N_keep_list(1:last_idx);
plot(plot_N_keep, plot_list);

title('Ground State Energy for 1D Hubbard Model U=2');
xlabel('Nkeep');
ylabel('Ground State Energy');
```

Ground State Energy for 1D Hubbard Model U=2
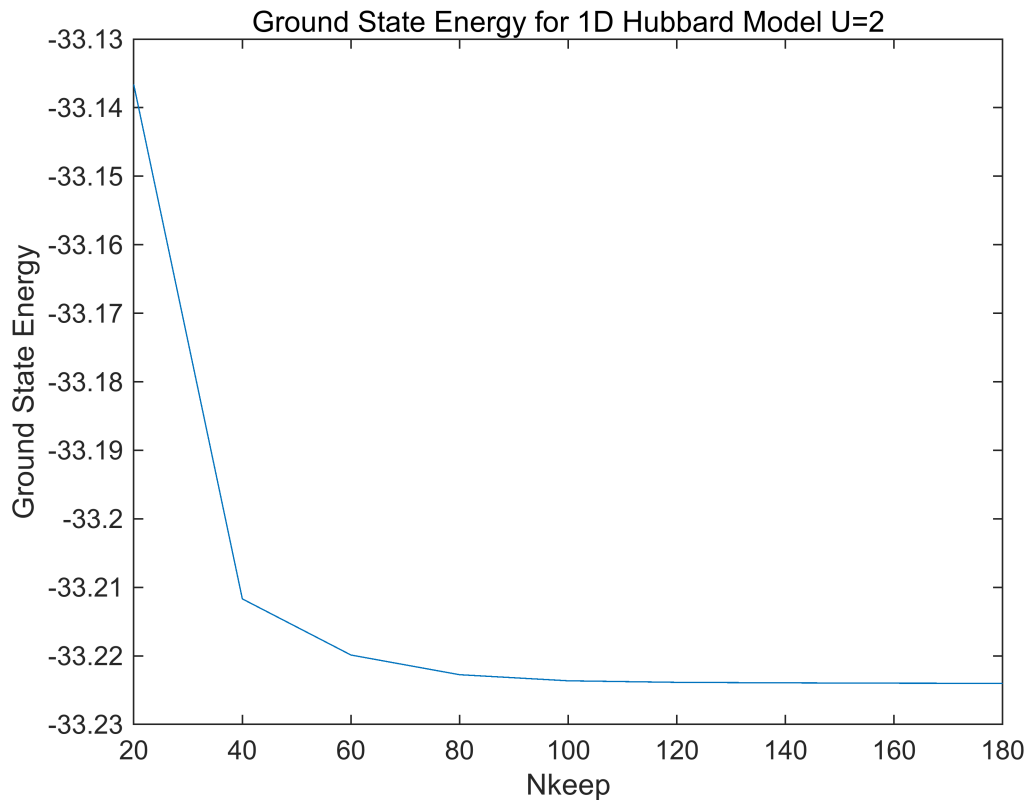
```
M0 = M; %to use the derived ground state
```

As N_keep was increased, the ground-state energy showed almost no change from N_keep = 180 onward, converging to a value of -33.22401.

Then, measure the double occupancy along the chain by computing it site by site, moving the orthogonality center through the chain using SVD.

```
%double occupancy

N = diag([0,0,0,1]) ; %double occupancy matrix
N_keep = N_keep_list(last_idx);
double_occupancy_list = zeros(1, L);

for i = L:-1:1 %from right to left, since M0 is left canonical
    X = contract(M0{i}, 3, [1, 2], conj(M0{i}), 3, [1, 2]);
    double_occupancy_list(i) = contract(X, 2, [1, 2], N, 2, [2, 1]);

    %move one site left
    if i > 1
        [U, S, M0{i}] = svdTr(M0{i}, 3, 1, N_keep, 0);
        US = contract(U, 2, 2, diag(S), 2, 1);
        M0{i-1} = contract(M0{i-1}, 3, 2, US, 2, 1, [1,3,2]);
    end
```
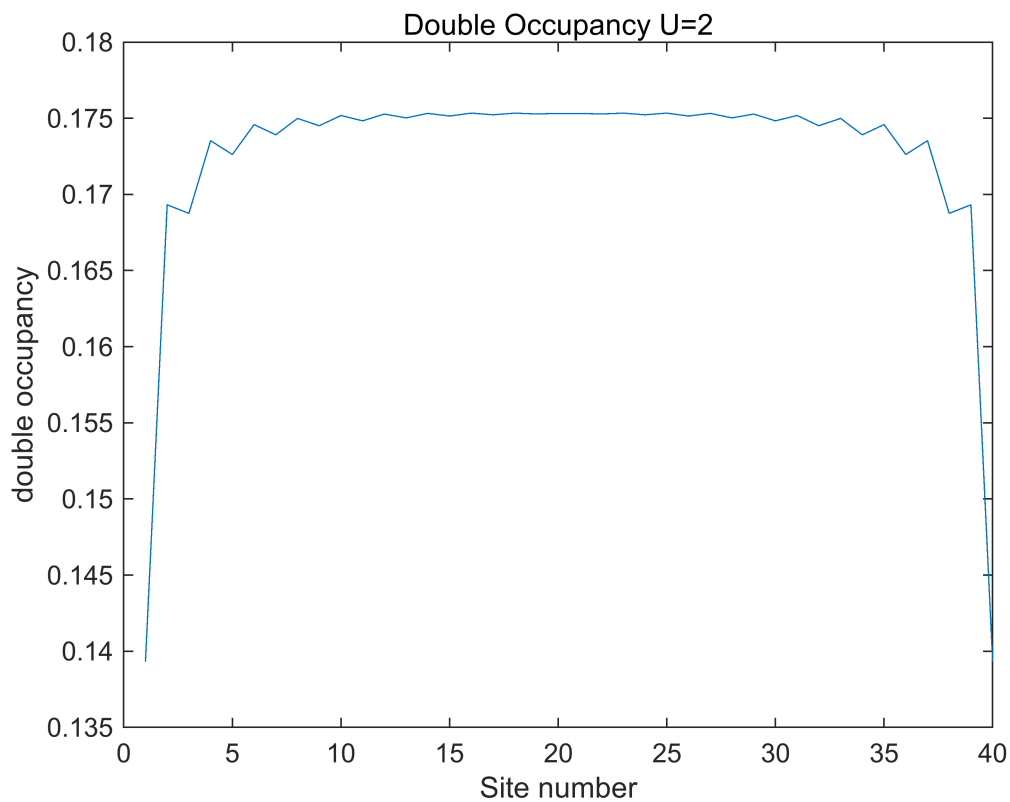
5

```
end
disp(double_occupancy_list);
```

      0.1393   0.1693   0.1688   0.1735   0.1726   0.1746   0.1739   0.1750   0.1745   0.1752   0.1748   0

```
figure;
plot(1:L, double_occupancy_list);
title('Double Occupancy U=2');
xlabel('Site number');
ylabel('double occupancy');
```


The double occupancies were approximately between 0.17 and 0.175, except at the edge sites, where the values dropped to around 0.14.

b. Repeat for U=10!

This time, I used 2 site update because 1 site update did not work well.

```
U = 10;
MPO = Hubbard_MPO(L, U, t);
E_G_list = zeros(length(N_keep_list));
threshold = 1e-6;

figure;
```

```matlab
for i = 1 : length(N_keep_list)
    N_keep = N_keep_list(i);
    [M, E_G, E_list] = my_dmrg(MPO, N_keep, N_sweep, 0, 2, L, physical_dim);
    E_G_list(i) = E_G;
    fprintf('Nkeep value : %d, E0 : %d', N_keep, E_G);
    if i>1 && abs((E_G - E_G_prev)/E_G_prev) < threshold
        last_idx = i;
        break;
    end
    E_G_prev = E_G;
end
```

```
25-05-20 15:40:26 | Sweep #1 of 10 (right -> left) : Energy = -9.883383
25-05-20 15:40:26 | Sweep #2 of 10 (left -> right) : Energy = -10.47715
25-05-20 15:40:26 | Sweep #3 of 10 (right -> left) : Energy = -10.51059
25-05-20 15:40:27 | Sweep #4 of 10 (left -> right) : Energy = -10.51552
25-05-20 15:40:27 | Sweep #5 of 10 (right -> left) : Energy = -10.5158
25-05-20 15:40:27 | Sweep #6 of 10 (left -> right) : Energy = -10.51589
25-05-20 15:40:28 | Sweep #7 of 10 (right -> left) : Energy = -10.51585
25-05-20 15:40:28 | Sweep #8 of 10 (left -> right) : Energy = -10.51589
25-05-20 15:40:28 | Sweep #9 of 10 (right -> left) : Energy = -10.51585
25-05-20 15:40:29 | Sweep #10 of 10 (left -> right) : Energy = -10.51589
Nkeep value : 20, E0 : -1.051589e+01
25-05-20 15:40:30 | Sweep #1 of 10 (right -> left) : Energy = -9.849963
25-05-20 15:40:31 | Sweep #2 of 10 (left -> right) : Energy = -10.47984
25-05-20 15:40:32 | Sweep #3 of 10 (right -> left) : Energy = -10.50947
25-05-20 15:40:33 | Sweep #4 of 10 (left -> right) : Energy = -10.51678
25-05-20 15:40:34 | Sweep #5 of 10 (right -> left) : Energy = -10.51795
25-05-20 15:40:35 | Sweep #6 of 10 (left -> right) : Energy = -10.51807
25-05-20 15:40:36 | Sweep #7 of 10 (right -> left) : Energy = -10.5181
25-05-20 15:40:38 | Sweep #8 of 10 (left -> right) : Energy = -10.5181
25-05-20 15:40:39 | Sweep #9 of 10 (right -> left) : Energy = -10.5181
25-05-20 15:40:40 | Sweep #10 of 10 (left -> right) : Energy = -10.5181
Nkeep value : 40, E0 : -1.051810e+01
25-05-20 15:40:42 | Sweep #1 of 10 (right -> left) : Energy = -9.954122
25-05-20 15:40:44 | Sweep #2 of 10 (left -> right) : Energy = -10.49911
25-05-20 15:40:46 | Sweep #3 of 10 (right -> left) : Energy = -10.51175
25-05-20 15:40:48 | Sweep #4 of 10 (left -> right) : Energy = -10.51582
25-05-20 15:40:50 | Sweep #5 of 10 (right -> left) : Energy = -10.51733
25-05-20 15:40:52 | Sweep #6 of 10 (left -> right) : Energy = -10.51808
25-05-20 15:40:55 | Sweep #7 of 10 (right -> left) : Energy = -10.51831
25-05-20 15:40:57 | Sweep #8 of 10 (left -> right) : Energy = -10.51834
25-05-20 15:40:59 | Sweep #9 of 10 (right -> left) : Energy = -10.51834
25-05-20 15:41:01 | Sweep #10 of 10 (left -> right) : Energy = -10.51834
Nkeep value : 60, E0 : -1.051834e+01
25-05-20 15:41:05 | Sweep #1 of 10 (right -> left) : Energy = -10.01947
25-05-20 15:41:10 | Sweep #2 of 10 (left -> right) : Energy = -10.48793
25-05-20 15:41:13 | Sweep #3 of 10 (right -> left) : Energy = -10.50476
25-05-20 15:41:16 | Sweep #4 of 10 (left -> right) : Energy = -10.51174
25-05-20 15:41:19 | Sweep #5 of 10 (right -> left) : Energy = -10.51502
25-05-20 15:41:22 | Sweep #6 of 10 (left -> right) : Energy = -10.51679
25-05-20 15:41:26 | Sweep #7 of 10 (right -> left) : Energy = -10.51768
25-05-20 15:41:29 | Sweep #8 of 10 (left -> right) : Energy = -10.51817
25-05-20 15:41:32 | Sweep #9 of 10 (right -> left) : Energy = -10.51832
25-05-20 15:41:35 | Sweep #10 of 10 (left -> right) : Energy = -10.51835
Nkeep value : 80, E0 : -1.051835e+01
```

```matlab
plot_list = E_G_list(1:last_idx);
```
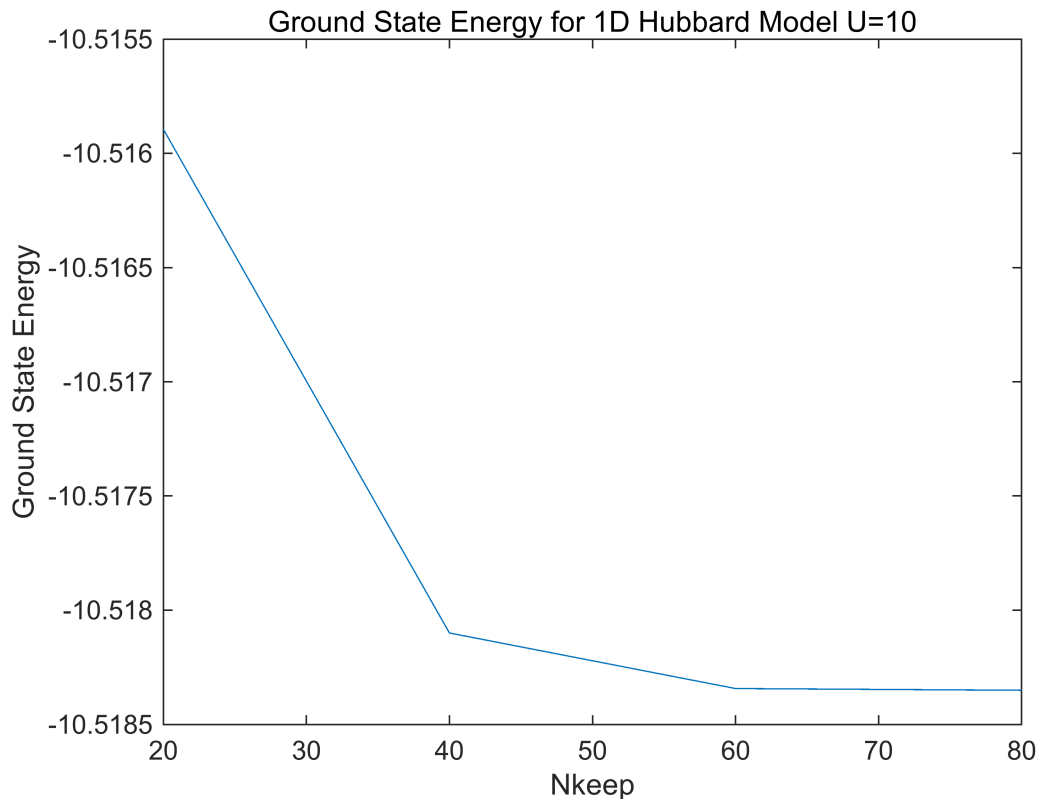
7

```
plot_N_keep = N_keep_list(1:last_idx);
plot(plot_N_keep, plot_list);

title('Ground State Energy for 1D Hubbard Model U=10');
xlabel('Nkeep');
ylabel('Ground State Energy');
```


Ground State Energy for 1D Hubbard Model U=10

```
M1 = M; %to use the derived ground state
```

This time, as N_keep was increased, the ground-state energy showed almost no change from N_keep = 80 onward, converging to a value of -10.51835.

When 1 site update was implemented, the ground state energy value did not converge as N_keep grew.

```
%double occupancy
N = [diag([0,0,0,1])] ; %double occupancy matrix
N_keep = N_keep_list(last_idx);
double_occupancy_list = zeros(1, L);

for i = L:-1:1 %from right to left, since M0 is left canonical
    X = contract(M1{i}, 3, [1, 2], conj(M1{i}), 3, [1, 2]);
    double_occupancy_list(i) = contract(X, 2, [1, 2], N, 2, [2, 1]);

    %move one site left
    if i > 1
```

```
        [U, S, M1{i}] = svdTr(M1{i}, 3, 1, N_keep, 0);
        US = contract(U, 2, 2, diag(S), 2, 1);
        M1{i-1} = contract(M1{i-1}, 3, 2, US, 2, 1, [1,3,2]);
    end
end
disp(double_occupancy_list);
```
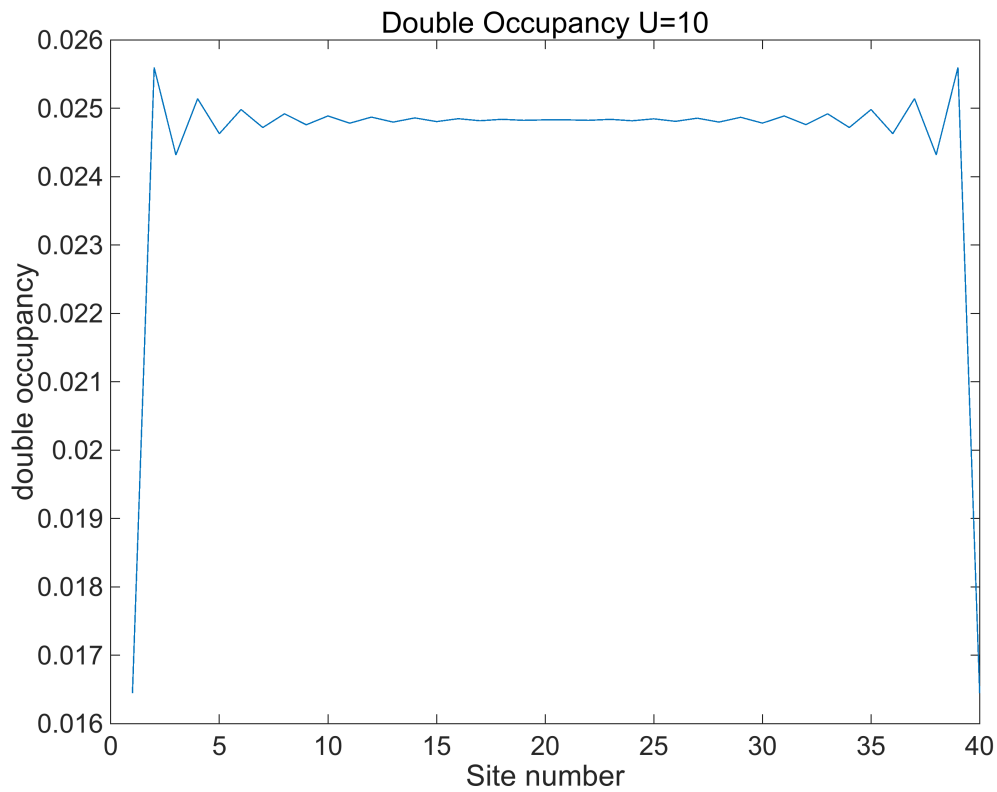
```
    0.0164    0.0256    0.0243    0.0251    0.0246    0.0250    0.0247    0.0249    0.0248    0.0249    0.0248    0
```

```
figure;
plot(1:L, double_occupancy_list);
title('Double Occupancy U=10');
xlabel('Site number');
ylabel('double occupancy');
```


This time, the double occupancy was much lower compared to the case of U = 2, with values around 0.025 except at the edges, where it was exactly 1/40. This suggests that a single pair of spin-up and spin-down electrons is uniformly distributed across all sites.