CPMC_Lab exercises report

icf

September 2017

1 Introduction

There are six problems in the Exercises and each question in the problem will be answered in four steps:

1) Pre-analysis
2) Matlab Program Modification
3) Input
4) Output
5) Discussion

Notice:
Calculation used the running parameters below if no special mention:
deltau=0.01;
N_wlk=100;
N_blksteps=200;
N_eqblk=3;
N_blk=10;
itv_modsvd=5;
itv_pc=10;
itv_Em=20;

2 Problem 1: Running the sample script

2.1 Question1: How much imaginary time is needed to equilibrate?

1) Pre-analysis

   Get the behavior (figure) of E vs. imaginary time (N_eqblk*N_blksteps*deltau) at the end of each bulk in "Equilibration phase".

   (When it comes to Equilibration Phase, the E wouldn't change or vibration around some value.)

2) Matlab Program Modification

   Calculate E in each bulk in the Equilibration phase: batchsample_deltau_icf.m

3) Input

   11.mat

   N_blksteps=40; N_eqblk=16; deltau=0.01;

4) Output

   11.fig

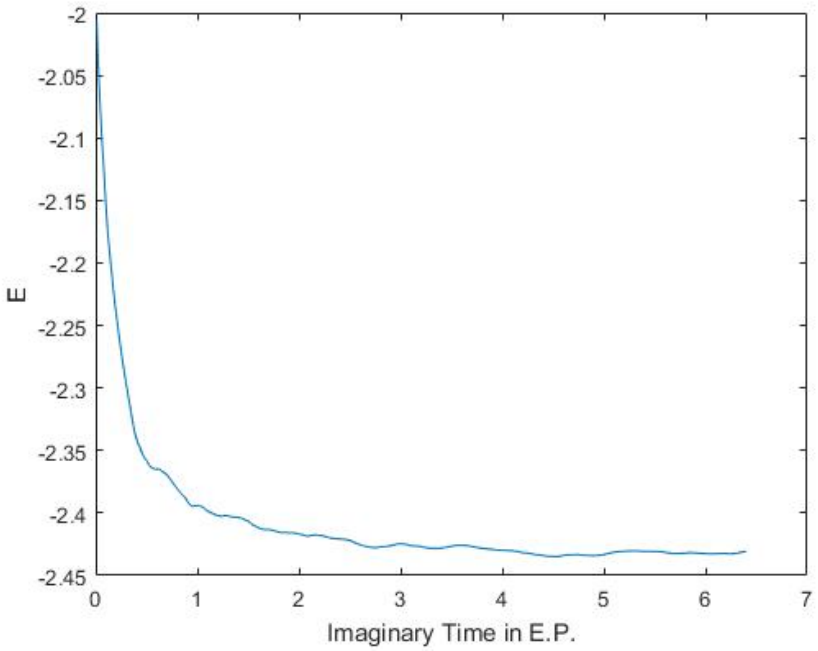


Figure 1: 11.fig: Mixed Energy vs. Imaginary Time, in Equilibration phase.

5) Discussion

   - The "E" above in 11.fig is "Mixed" Energy which used to describe the "Equilibration Phase Stability" and the better method to describe the "Equilibration Phase Stability" is $||\phi_i > -|\phi_{i+N} > |^2$ where $\{|\phi_i >\}$are states after each bulk and $N = 1, 2, ...$
   - N_eqblk, N_blksteps and deltau affect the state propagation together as "imaginary time = N_eqblk*N_blksteps*deltau ".
   - **According to the Output, imaginary time >= 4 is chosen to be the imaginary time to include an "Equilibration Phase".**

2.2 Question2: after get an equilibration phase, get the minimum length of a reliable N_blksteps.

1) Pre-analysis

   Change N_blksteps with fixed imaginary time >= 4 in equilibration phase.

   The reliable "N_bliksteps" lead to an small and stable "E_err" in Measurement phase .

2) Matlab Program Modification

   batchsample.m for different N_blksteps.

3) Input

   N_blksteps=[40:20:320];

4) Output

   14.fig

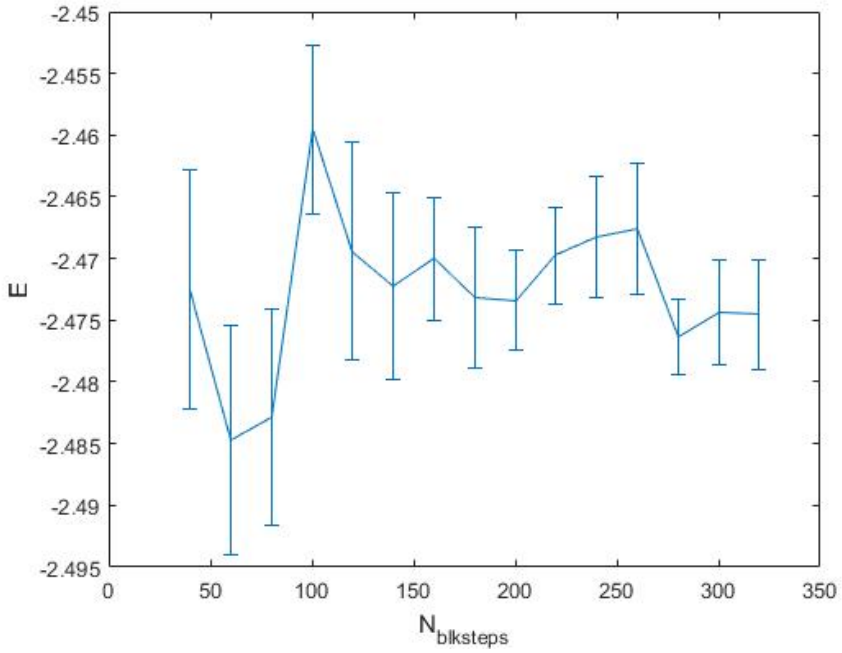


Figure 2: 14.fig: E, E_err vs. N_blksteps with fixed imaginary time >= 4 in equilibration phase.

5) Discussion

System	(kx,ky)	E_0	E_c	Data
2*1	(+0.0819,0)	-2.44260	-2.44215	15.mat
4*1	(+0.0819,0)	-2.11671	-2.10726	16.mat
8*1	(+0.0819,0)	-4.60591	-4.61115	17.mat
2*4	(+0.0819,-0.6052)	-12.1210	-12.12566	18.mat
3*4	(+0.02,0.04)	-13.9918	-13.99065	19.mat
4*4	(0,0)	-19.58094	-19.58320	20.mat

Table 1: E_c is calculated result and E_0 is Ground state Energy.

When N_blksteps more than 200, then E_err become stable and reliable. (Although there should be more accurate if N_blksteps goes far like 1000, as an exercise it is not necessary to spend to much time in calculation.)

2.3 Question3: using "correct" parameters, compare the results in Table 1

1) Input

   batchsample_Lx_Ly_icf.m;

   15.mat;16.mat;17.mat;18.mat;19.mat;20.mat;

2) Output

   Table 1.

3 Problem 2: Controlling the basic run parameters

3.1 Question1: E vs. deltau (the sliced length) in comparable statistics

1) Pre-analysis

   Change deltau with deltau*N_blksteps and deltau*itv_em fixed.

2) Matlab Program Modification

   batchsample_deltau_icf.m

3) Input

   21.mat

4) Output

   21.fig

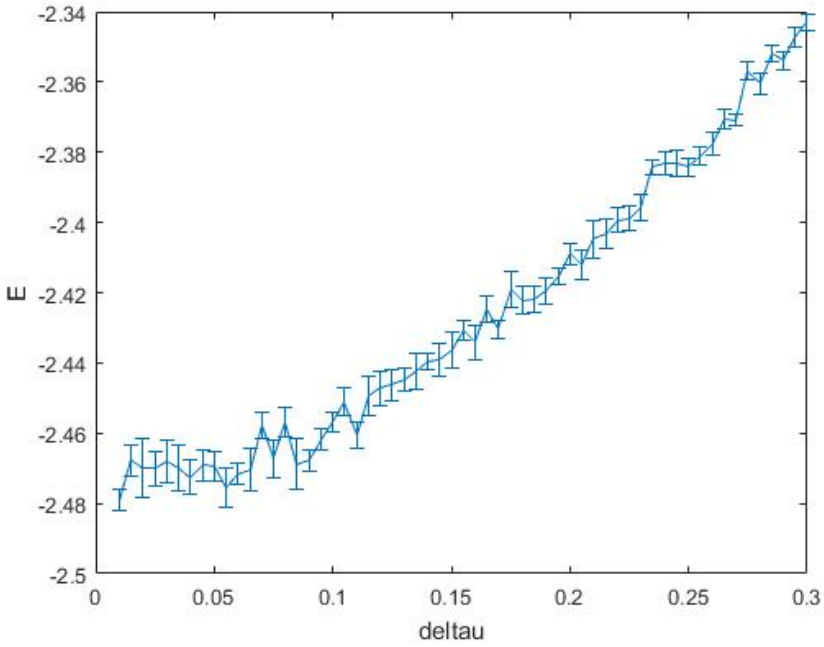


Figure 3: 21.fig: E vs. deltau (the sliced length) with deltau*N_blksteps and deltau*itv_em fixed.

5) Discussion

   - The smaller deltau is, the smaller E is.
   - **Smaller deltau lead to a larger E_err and need more calculation time,** $deltau = 0.01$ **for all calculation here for convinence**.
   - A part of the difference between state calculated by CPMC and the real Ground state is from the slice process.

3.2 Question3: E_err vs. N_wlk*bulk

1) Pre-analysis

   Change N_wlk (The number of walker) with N_wlk*N_blk and N_wlk*N_eqblk fixed.

2) Matlab Program Modification

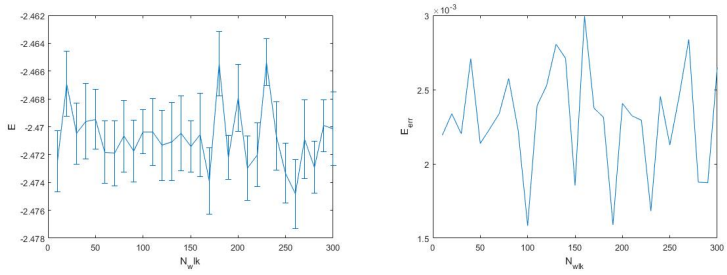
   batchsample_N_wlk_icf.m

3) Input

   22.mat

4) Output

   22.fig;22_2.fig;



(a) 22.fig: E, E_err vs. N_wlk (The number of walker)

(b) 22_2.fig: E_err vs. N_wlk

Figure 4: The Error change little with fixed N_wlk*N_blk and N_wlk*N_eqblk.

5) Discussion

   If N_wlk*N_blk and N_wlk*N_eqblk are fixed, the accuracy of E (E_err) wouldn't change much, which means "time" and "space" are equivalent in CPMC process.

4 Problem3: Calculating E_K and E_V separately and compare with Table3

1) Pre-analysis

   AS

$$E\_V =< \phi(U)|U\frac{\mathrm{d}H(U))}{\mathrm{d}U}|\phi(U) >= U\frac{\mathrm{d}E(U)}{\mathrm{d}U} \equiv U \lim_{\Delta U\to 0} \frac{E(U+\Delta U)-E(U-\Delta U)}{2\Delta U}$$

   And

$$E\_V =< \phi(t_x,t_y)|t_x\frac{\mathrm{d}H(t_x,t_y))}{\mathrm{d}t_x}+t_y\frac{\mathrm{d}H(t_x,t_y))}{\mathrm{d}t_y}|\phi(t_x,t_y) >= t_x\frac{\mathrm{d}E(t_x,t_y)}{\mathrm{d}t_x}+t_y\frac{\mathrm{d}E(t_x,t_y)}{\mathrm{d}t_y}$$

$$\equiv t_x \lim_{\Delta t_x\to 0} \frac{E(t_x+\Delta t_x,t_y)-E(t_x-\Delta t_x,t_y)}{2\Delta t_x}+t_y \lim_{\Delta t_y\to 0} \frac{E(t_y+\Delta t_y,t_x)-E(t_y-\Delta t_y,t_x)}{2\Delta t_y}$$

   There are two steps:

   1. Find a reliable and minimum $\Delta U \equiv deltaU$ and corresponding Δt_x, Δt_y according to the E_err for a set of different $deltaU$. (E_err is $std(E\_V(i,:))/\sqrt{N\_loop}$ used to describe the stability of E with each $deltaU$ and N_loop is the times of calculations under the same deltaU.)
   2. Use the H.F. Theorem to calculate E_V and E_K.

2) Matlab Program Modification

   sample_E_V_icf.m;

   sample_E_K_icf.m;

3) Input

   E_V,E_V_err vs. deltaU : 27.mat;

   E_K,E_K_err vs. deltaU : 25.mat;

   28_1.mat;28_2.mat;28_3.mat;28_4.mat;28_5.mat;28_6.mat;

4) Output

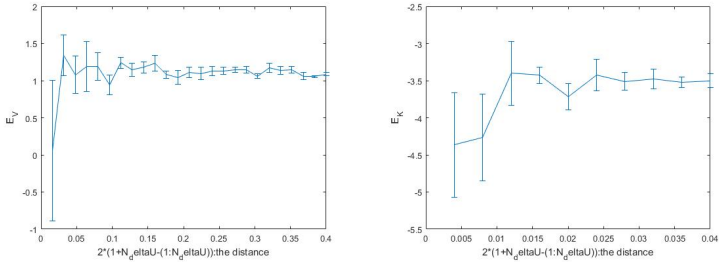
   E_V,E_V_err vs. deltaU : 27.fig;

   E_K,E_K_err vs. deltaU : 25.fig;

   Table 2.

5) Discussion

   The reliable deltaU for U, t_x and t_y may be different but $deltaU = 0.08$ in all calculation related here for convenience.



(a) 27.fig: E_V, E_V_err vs. 2*deltaU (b) 25.fig: E_K, E_K_err vs. 2*deltaU

Figure 5: Large *deltaU* lead to stable derivative.

System	(kx,ky)	$< K >$	$< V >$	$< K >_c$	$< V >_c$	Data
2*4	(+0.0819,-0.6052)	-13.7778	1.65680	-13.7779	1.6176	28_4.mat $28_1.mat$
3*4	(+0.02,0.04)	-15.2849	1.29311	-15.2520	1.2917	28_5.mat $28_2.mat$
4*4	(0,0)	-22.5219	2.94100	-22.4981	2.9079	28_6.mat $28_3.mat$

Table 2: $< V >_c$, $< K >_c$ is calculated results with H.F. Theorem and $< V >$, $< K >$ are Ground State Kinetic and Potential Energy.

5 Problem4: The Hydrogen molecule

5.1 Question1: Compare E vs. U with exact solution

1) Matlab Program Modification
   batchsample_U.m;

2) Input
   29.mat;

3) Output
   29.fig;

5.2 Question2: plot E_V vs. U and E_K vs. U

1) Matlab Program Modification
   batchsample_E_K.m;
   batchsample_E_V.m;

2) Input
   E_V,E_V_err vs. U : 31.mat;
   E_K,E_K_err vs. U : 54.mat;

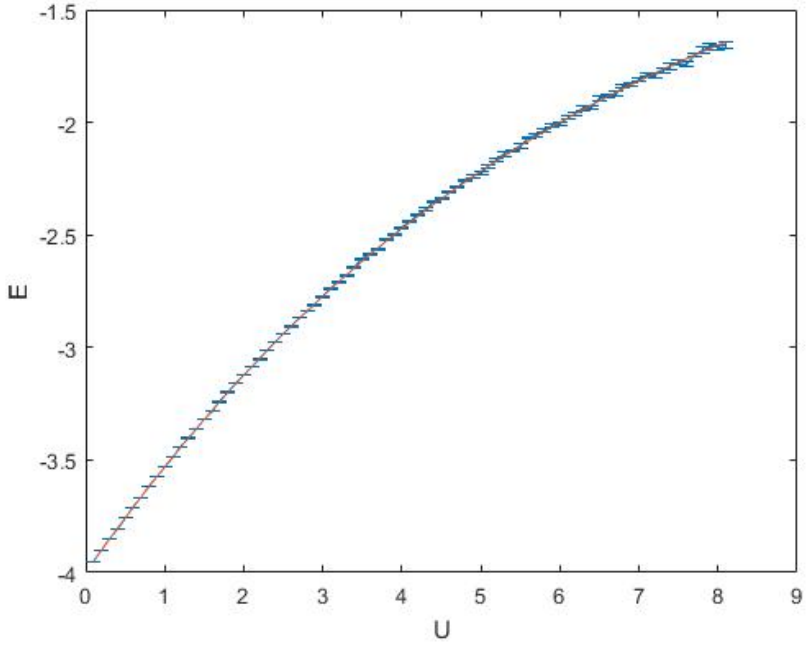
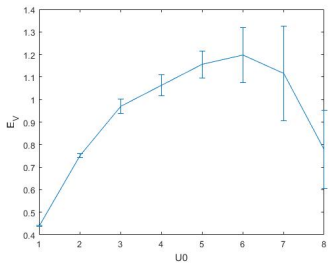


Figure 6: 29.fig: red curve is analytic solution and blue points are CPMC results.

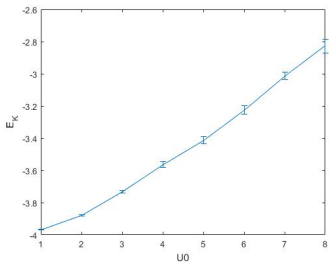
3) Output

E_V,E_V_err vs. U : 31.fig;

E_K,E_K_err vs. U : 54.fig;



(a) 31.fig: E_V, E_V_err vs. U, deltaU=0.08



(b) 54.fig: E_K, E_K_err vs. U, deltaU=0.08

Figure 7: E_V, E_V_err and E_K, E_K_err increase with increasing U

4) Discussion

According to the output figure, E_V, E_V_err and E_K, E_K_err become larger with increasing U.

- The E_V increase because U increase.
- The E_K increase because electrons are harder to move due to an increasing U.
- The E_V_err and E_K_err increase because the Error of derivative $\propto \frac{\Delta E}{\Delta U}$ where ΔE is the error from QMC process considered as an linear function of $U^2 \approx Ue^{aU}$ (E_V_err: 51.fig,51.mat.) (The e^{aU} in the estimation comes from $[e^{H_K}, e^{H_V}]$ and the U in Ue^{aU} from $H = ... + U\sum_i n_i n_i$).
  E_V_err is linear with $\Delta U \equiv deltaU$ (E_V, E_V_err: 49.fig, 49.mat with deltaU=0.04 and 50.fig, 50.mat with deltaU=0.16. However when deltaU becomes lager the estimate of derivative becomes less accurate.)
- And there is still a problem that: the huge difference between E_K_err and E_V_err.

5.3 Question3: the double occupancy and the correlation function vs. U

1) Pre-analysis

Consider

$$H' = K+V' = -t_x \sum_{<i,j>,\sigma} (c^\dagger_{i,\sigma} c_{i,\sigma} + c.c.) + U_1(n_{1,up}n_{1,dn}) + U_{12}(n_{1,up}n_{2,dn}) + U\sum_i (n_{i,up}n_{i,dn})$$

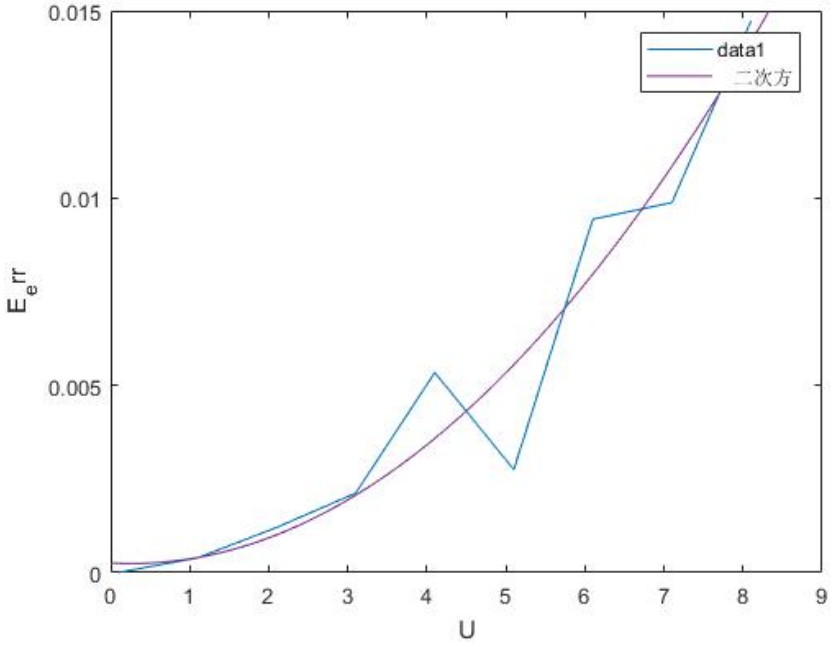
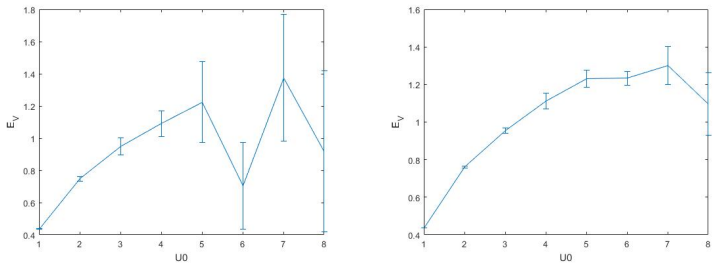


Figure 8: 51.fig: The Error of E (ΔE) vs. U is linear with $U^2 \approx Ue^{aU}$



(a) 49.fig: E_V, E_V_err vs. U, deltaU=0.04

(b) 50.fig: E_V, E_V_err vs. U, deltaU=0.16

Figure 9: E_V_err is linear with $\Delta U \equiv deltaU$

, according to H.F. Theorem:

$$< n_{1,up} n_{1,dn} >= \frac{\mathrm{d} < \phi_0(U_1)|H'(U_1)|\phi_0(U_1) >}{\mathrm{d}U_1} = \frac{\mathrm{d} < \phi_T|H'(U_1)|\phi_0(U_1) >}{\mathrm{d}U_1}$$

$$< n_{1,up} n_{2,dn} >= \frac{\mathrm{d} < \phi_0(U_{12})|H'(U_{12})|\phi_0(U_{12}) >}{\mathrm{d}U_{12}} = \frac{\mathrm{d} < \phi_T|H'(U_{12})|\phi_0(U_{12}) >}{\mathrm{d}U_{12}}$$

There are three steps:

1. Modefy the propagate process to get the Ground state of $H'(U_1, U_{12})$.
2. Modefy the measure process to get the mixed measurement of $H'(U_1, U_{12})$.
3. Calculate the difference over deltau (derivative) around $U_1 = U$ and $U_{12} = 0$.

2) Matlab Program Modification

batchsample_NiNi_icf.m;

initialization_NiNi.m;

CPMC_Lab_NiNi.m;

stepwlk_NiNi.m;

measure_NiNi.m;

batchsample_N1N2_icf.m;

initialization_N1N2.m;

CPMC_Lab_N1N2.m;

stepwlk_N1N2.m;

measure_N1N2.m;

3) Input

$< n_{1,up} n_{1,dn} >$: 56.mat;

$< n_{1,up} n_{2,dn} >$: 57.mat;

4) Output

$< n_{1,up} n_{1,dn} >$: 56.fig;

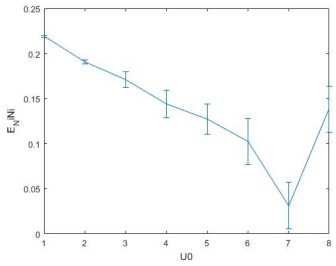
$< n_{1,up} n_{2,dn} >$: 57.fig;

5) Discussion

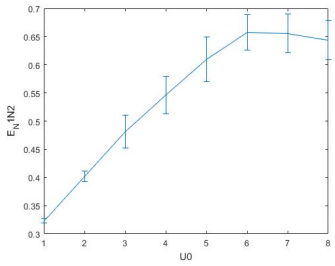
- $|\phi_0 >$ must be the ground state of H' or

$$< \phi_T|H'|\phi_0 > \neq < \phi_0|H'|\phi_0 >$$

  . (Ignore the normalization.)
- **As U increasing, it become harder for electrons to stay together so the double occupancy decrease. For the same reason, the correlation function increase.**



(a) 56.fig: $< n_{1,up} n_{1,dn} >$ vs. U



(b) 57.fig: $< n_{1,up} n_{2,dn} >$ vs. U

Figure 10:

6 Problem5: Ground state Energy of a chain

1) Input

   38.mat;

2) Output

   55.fig;

5) Discussion

7 Problem6: Other correlation functions

1) Pre-analysis

   Modefy the measurement process.

2) Matlab Program Modification

   batchsample_U_mixed.m; CPMC_Lab_mixed.m; measure_mixed.m; stepwlk_mixed.m;

3) Input

   40.mat;41.mat;42.mat;

4) Output

   Table 3, Table 4.

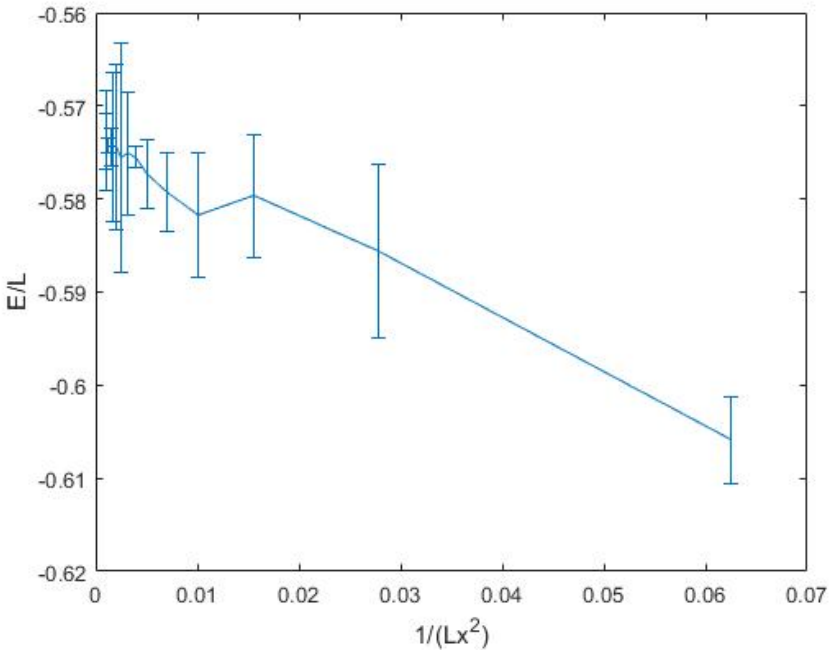


Figure 11: 55.fig: E/L_x vs. $1/L_x^2$, The Ground State Energy per site in the half-filled chain system converge at a point with increasing L_x

System	(kx,ky)	$< K >$	$< V >$	$< K >_{mixed}$	$< V >_{mixed}$	Data
2*4	(+0.0819,-0.6052)	-13.7778	1.65680	-14.3892	2.2609	40.mat
3*4	(+0.02,0.04)	-15.2849	1.29311	-15.9954	2.0002	41.mat
4*4	(0,0)	-22.5219	2.94100	-24	4.4205	42.mat

Table 3: $< V >_{mixed}$, $< K >_{mixed}$ are calculated mixed results of Kinetic and Potential Energy and $< V >$, $< K >$ are Ground State Kinetic and Potential Energy.

System	(kx,ky)	$< c1c2 >_{mixed}$	$< s1s2 >_{mixed}$	$< c1c2c >_{mixed}$	Data
2*4	(+0.0819,-0.6052)	0.3821	-0.0405	0.3890	40.mat
3*4	(+0.02,0.04)	0.2408	-0.0419	0.2460	41.mat
4*4	(0,0)	0.1861	-0.024	0.3881	42.mat

Table 4: $< c1c2 >_{mixed}$, $< s1s2 >_{mixed}$, $< c1c2c >_{mixed}$ are calculated mixed results of One body spin up density matrix, spin-spin correlation function and the charge-charge correlation function for $i = 1$, $j = 2$.