Quantum Monte Carlo Methods at Work for Novel Phases of Matter

SSE TUTORIAL II

Projector QMC for Heisenberg model

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TASKS TO DO (DAY II)

- Tour inside **probasic.f90**
- Test correction of the program
- Test convergence of the program
- Measurement of spin-spin correlation **C(r)** (transition graph)
- Tutorial III (JQ Chain)

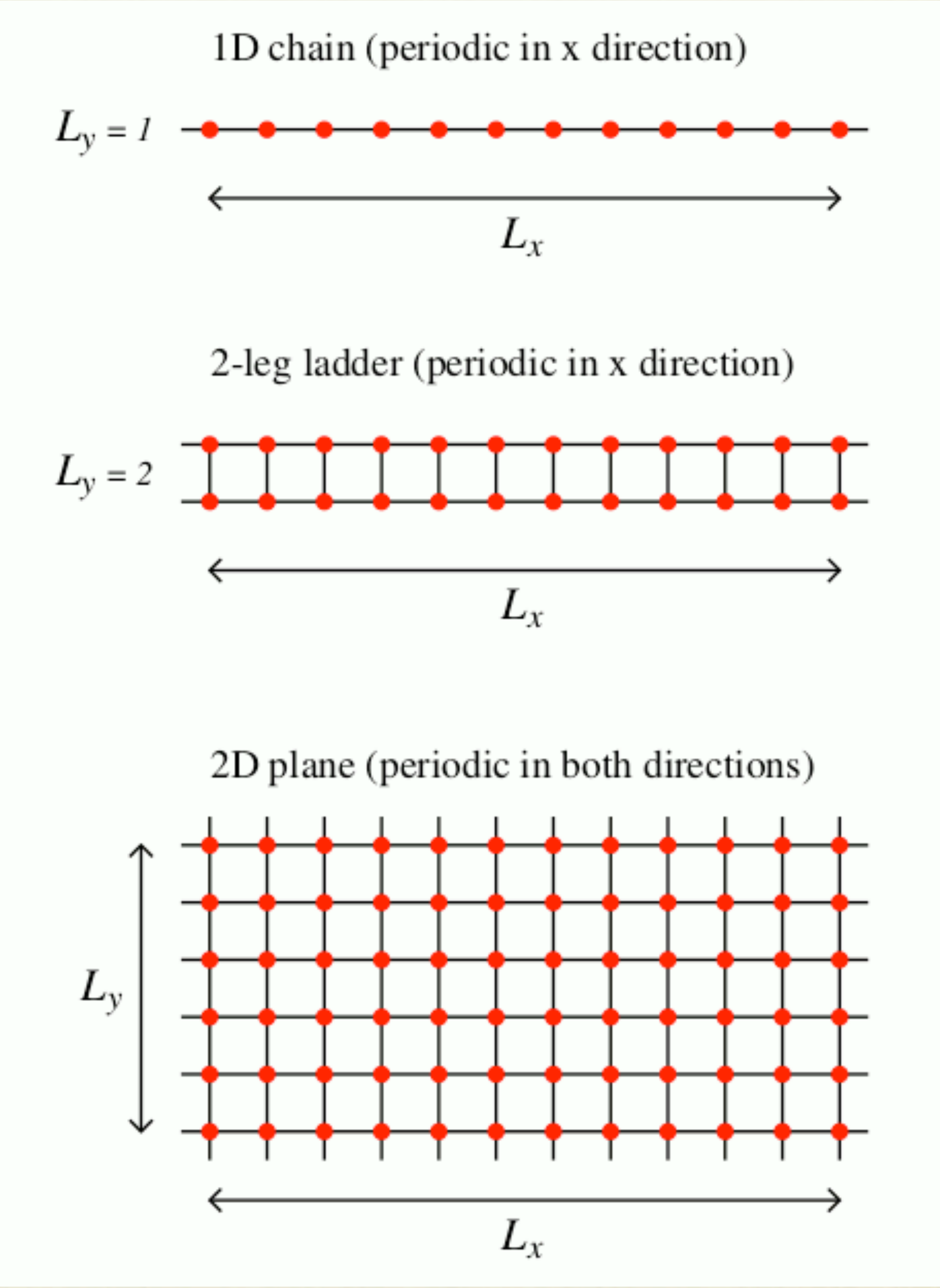
TOUR INSIDE PROBASIC.F90

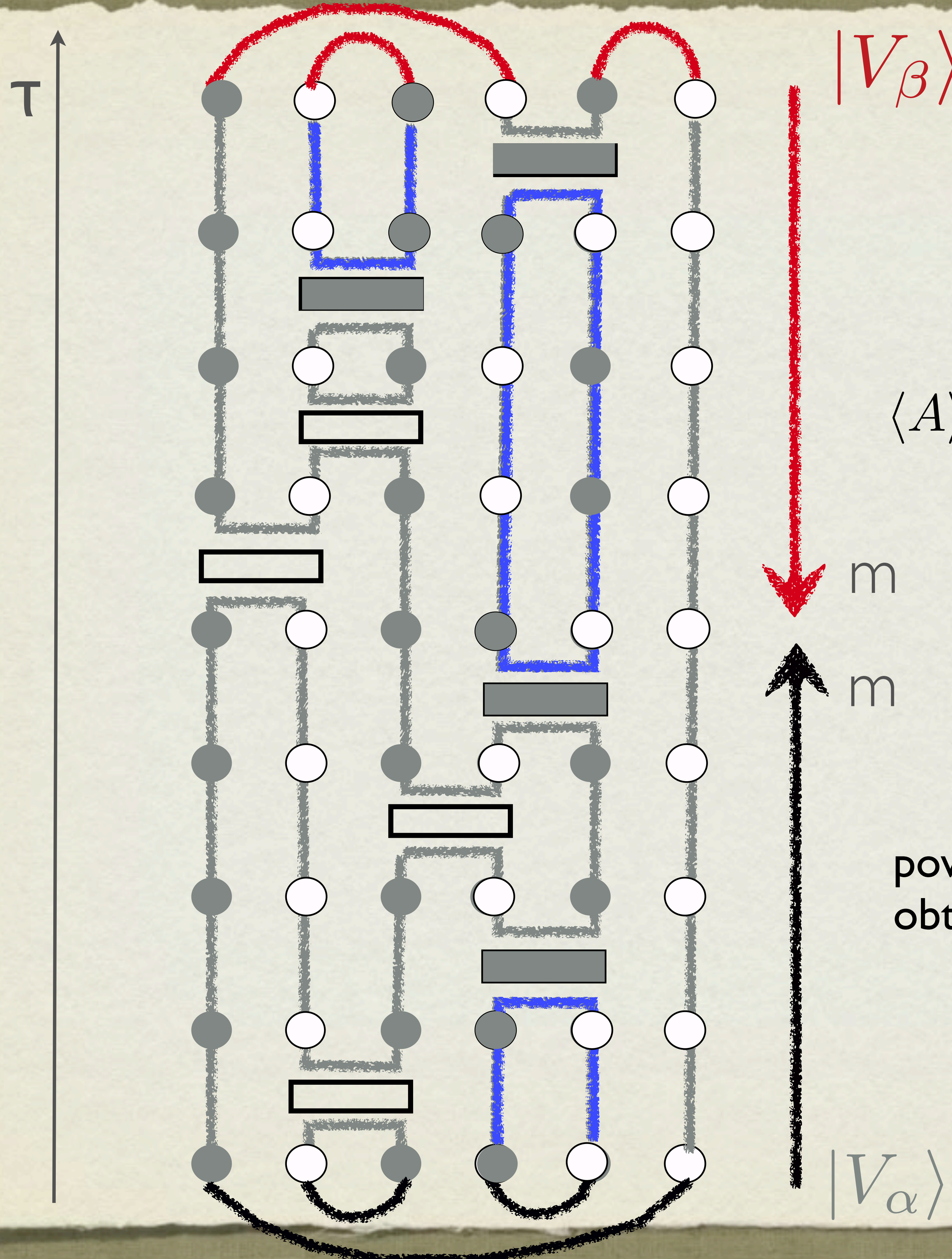
- The program can be found at:

http://physics.bu.edu/~sandvik/trieste12/

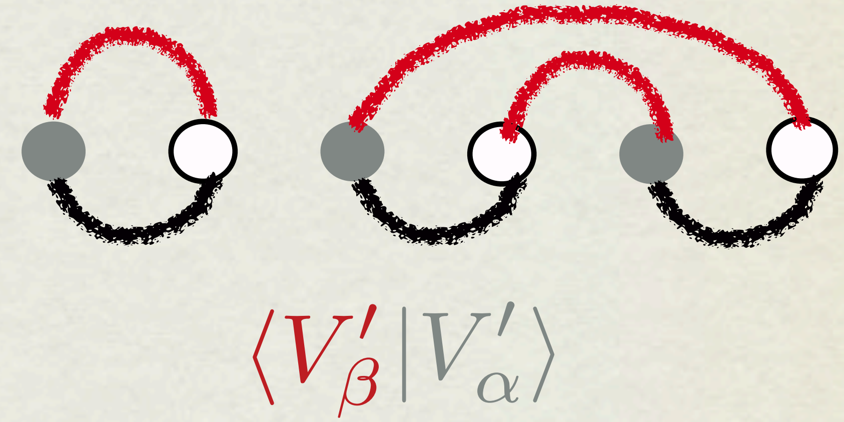
- Heisenberg Model

$$H = \sum_{<i,j>} J\mathbf{S_i} \cdot \mathbf{S_j}$$

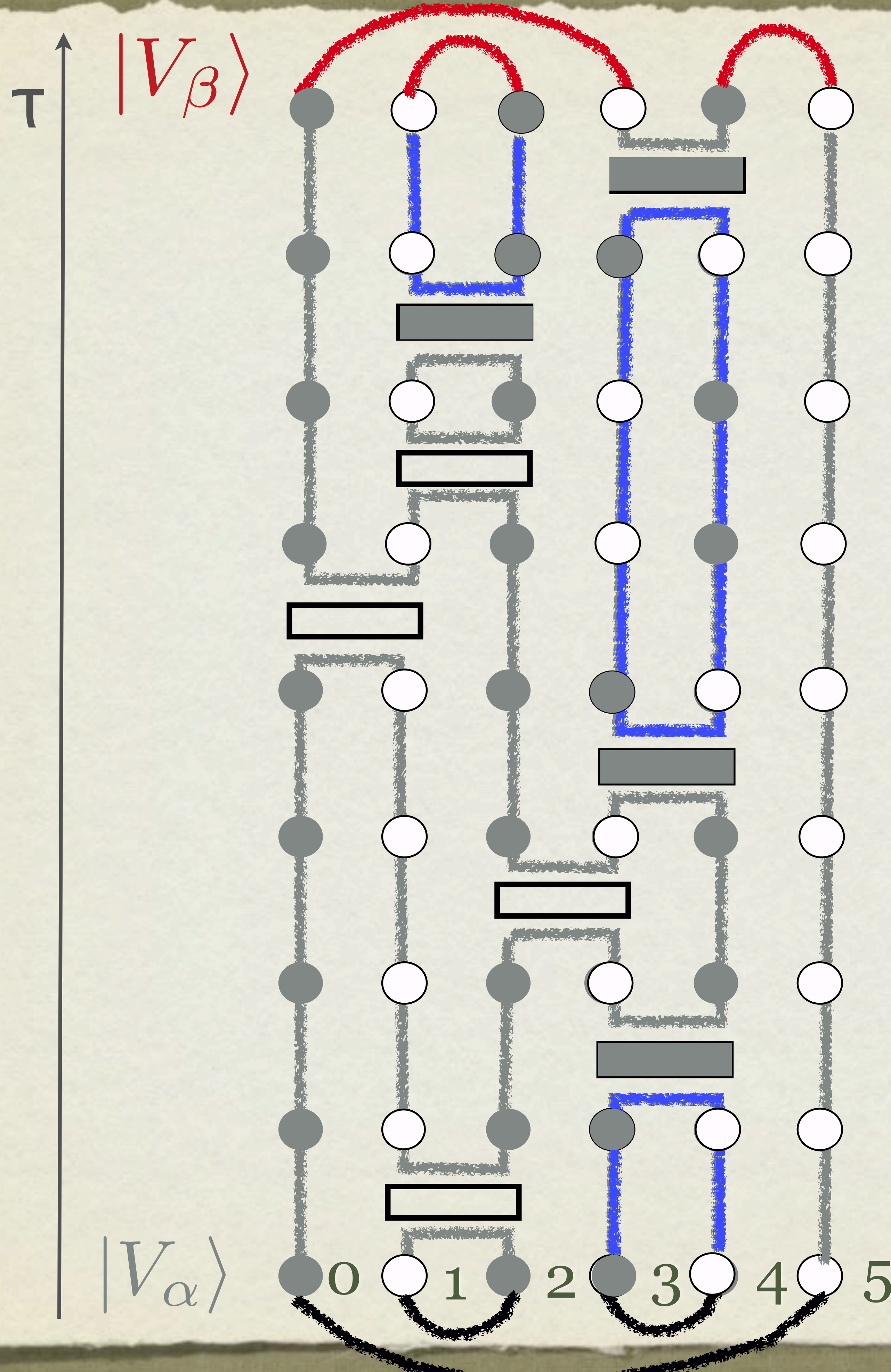




$$\langle A\rangle = \frac{\langle\psi_1|(-H)^m A(-H)^m|\psi_2\rangle}{\langle\psi_1|(-H)^{2m}|\psi_2\rangle}$$



power m should be large enough to obtain ground states



m	oper(m)				
7		1	1	1	7
6			1	1	3
5			1	0	2
4				0	0
3		1	1	1	7
2		1	0	0	4
1		1	1	1	7
0			1	0	2

GET STARTED

- Download the program to Projection QMC directory (e.g. ~/qmc)
- Generate input file **read.in** and random number seed file **seed.in** in the same directory.
- Compile program with **g95/gfortran**
  - **gfortran -O probasic.f90**
- run **./a.out**

read.in

```
lx, ly, mm
init, nbins, mstps, istps
```

seed.in

```
an integer
```

lx,ly : Lattice size in x and y direction
mm : Projection power = mm*N/2
init : Initial configuration (init=0, start from beginning)
nbins : Number of bins (averages written to file 'cor.dat' after each bin
msteps : Number of MC sweeps in each bin (measurements after each sweep)
isteps : Number of MC sweeps for equilibration (no measurements)

A QUICK TEST

Note, real power = 64*N/2

read.in

```
32   1   64
0   10   10000 10000
```

(takes ~14 seconds on macbook air)

Output files: cor.dat [r and C(r)]

- Calculate error bars
  - compile prores.f90 **gfortran -o b.out -O prores.f90**
  - run **./b.out**

c.dat

r	C(r) ...	error
0	0.75000000	0.00000000
1	0.44391200	0.00021255
2	0.18286811	0.00033708
3	0.15290305	0.00027568
4	0.10635810	0.00026413
5	0.09644702	0.00027540
6	0.07733501	0.00024390
7	0.07295753	0.00020930
8	0.06266420	0.00024304

TEST OF CORRECTNESS

COMPARE C(R) WITH MEASUREMENTS IN SSE

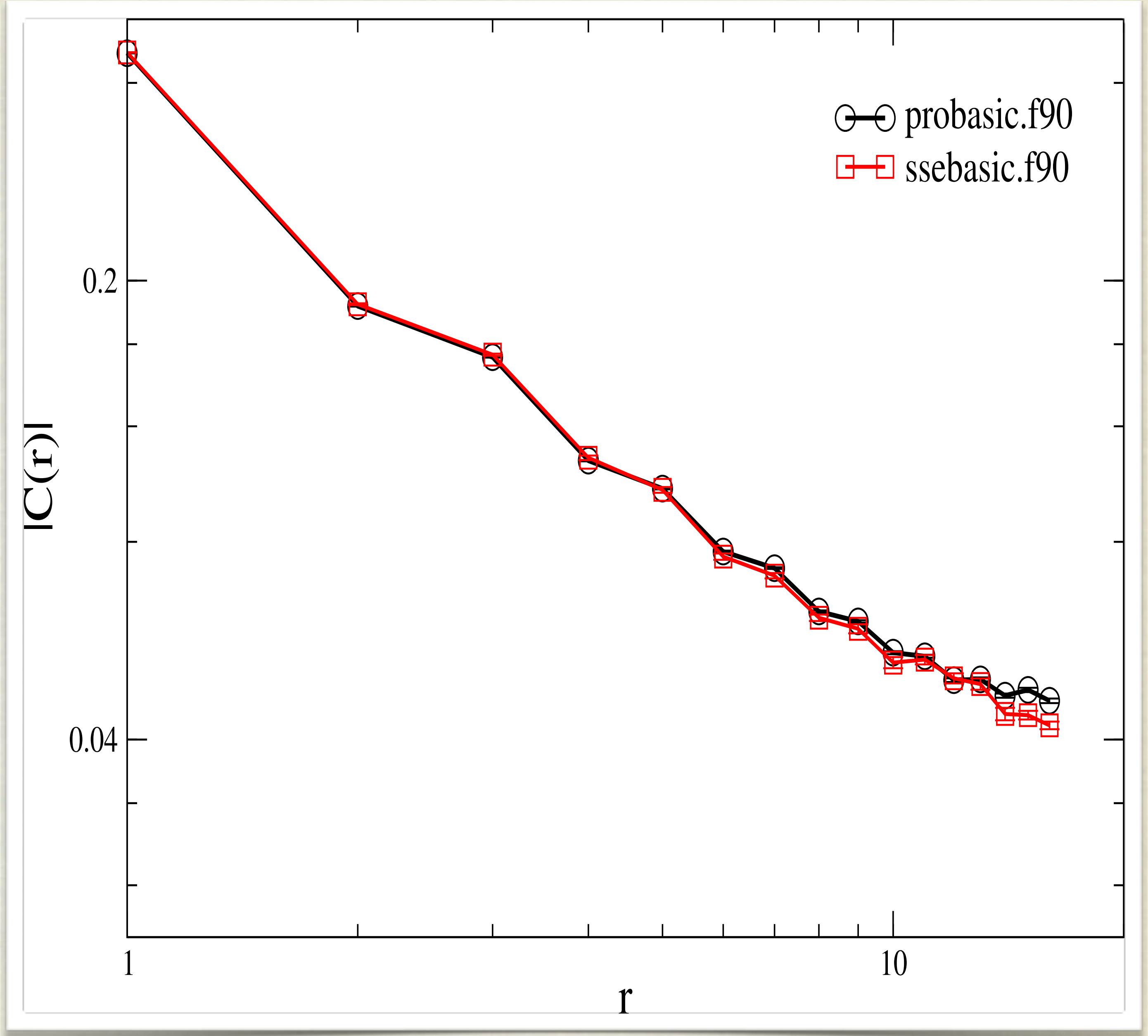
TASK TO DO

- Compare $3C^z(r)$ calculated by SSE and **C(r)** calculated by PMC

Suggested Parameters (challenge large L)
L=32
β=64 (sse)
mm=64 (projector)
bin=10 mcstep=1000

- Compare (mc=10^5, ~30 mins)

$3C^Z(L/2)$	0.04550466	0.00036189
C(L/2)	0.04552031	0.00010459



TEST OF CONVERGENCE

TASK TO DO

- At <u>a fixed r</u> (e.g. r=L/2), plot **C(L/2)** versus **mm**
- Observe the convergence behavior in 1D and 2D

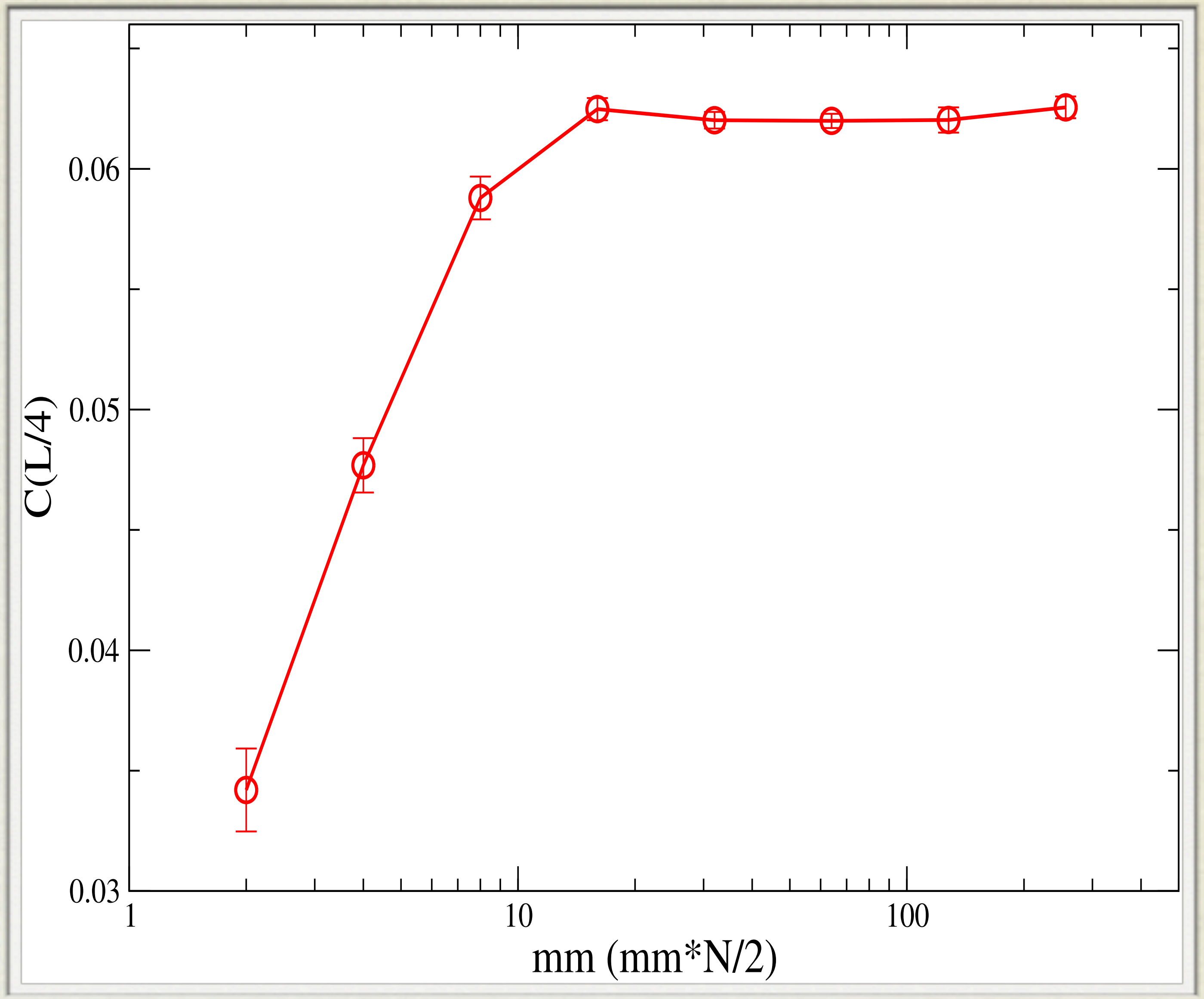
Question to think about:

Can you predict the sufficient power if you know the system size N?

hint:

$$(-H)^m|\psi\rangle = c_0(-E_0)^m[|0\rangle + \sum_{m=1}^{\Lambda-1}\frac{c_n}{c_0}(\frac{E_n}{E_0})^m|n\rangle]$$

singlet gap $\Delta \propto 1/L$

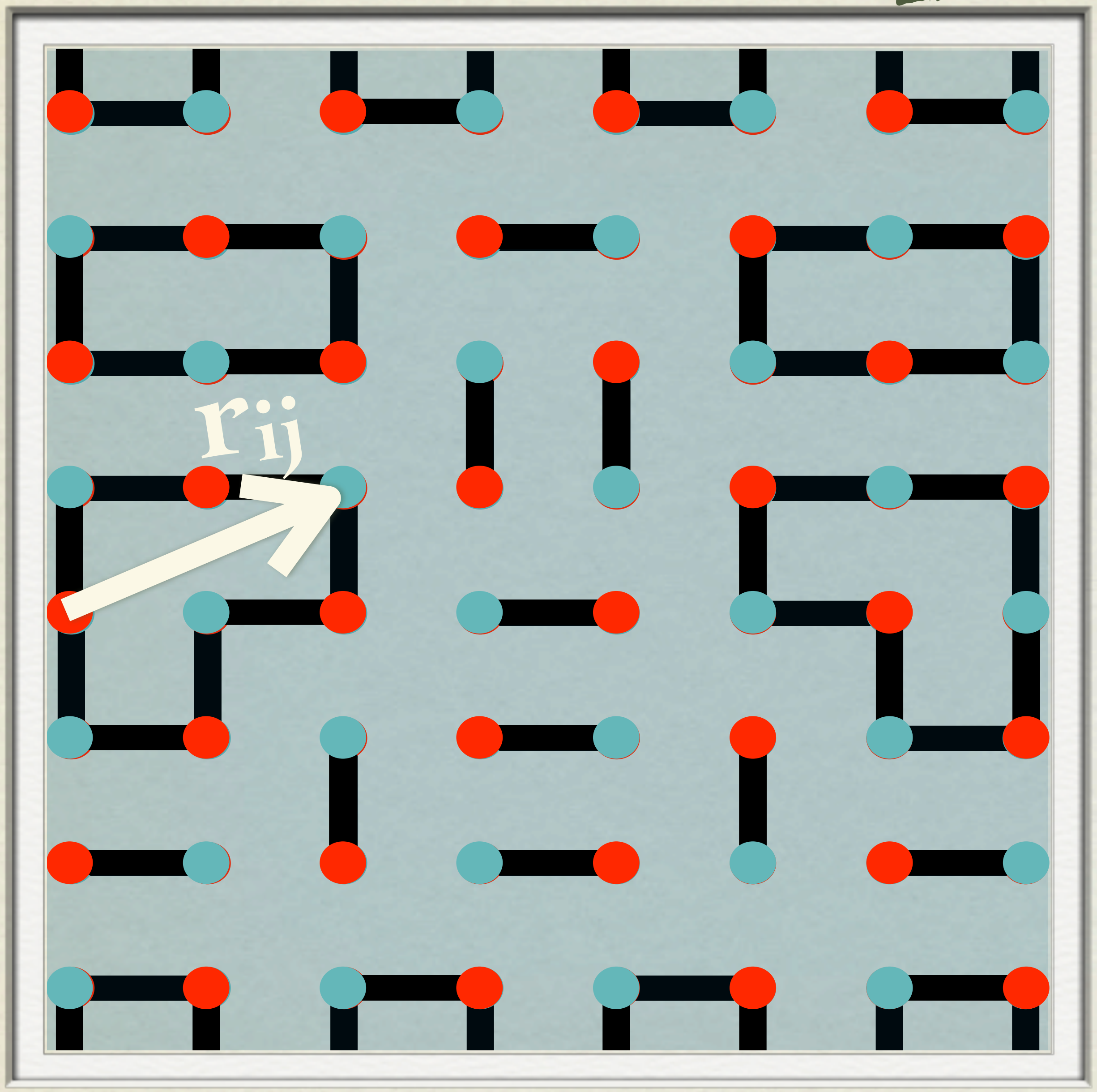


1D Chain, L=32, bin=10, mstps=10^4

(takes a couple of minutes)

answer: m ~ NL

MEASUREMENT OF C(R) --- TRANSITION GRAPH

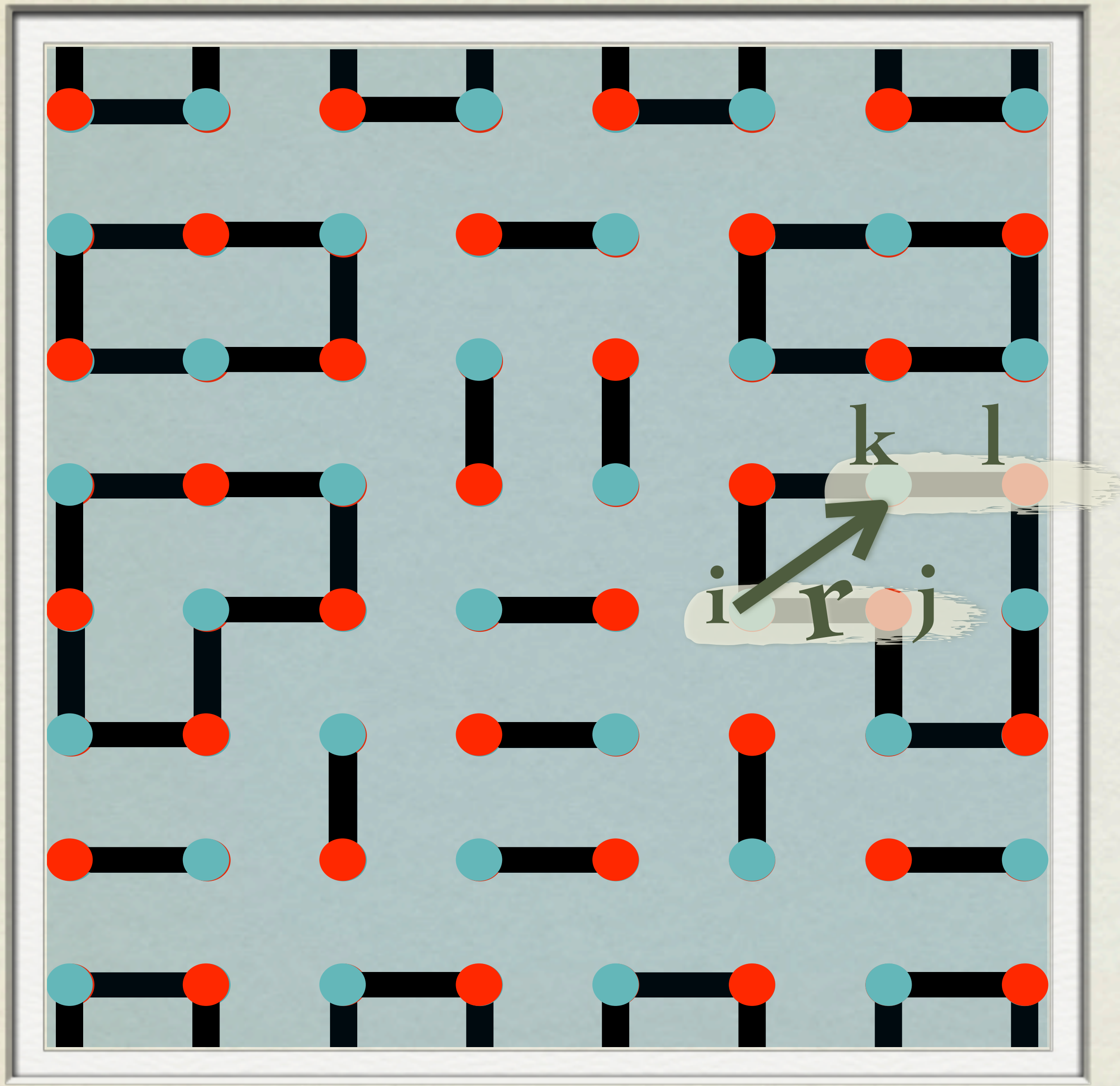


$$C(\mathbf{r_{ij}}) = \frac{\langle V_\beta | \mathbf{S}_i \cdot \mathbf{S}_j | V_\alpha \rangle}{\langle V_\beta | V_\alpha \rangle} = \begin{cases} 0, & (i)_L (j)_L \\ \frac{3}{4}\phi_{ij}, & (i,j)_L \end{cases}$$

$$\phi_{ij} = \begin{cases} +1 & \text{i , j are on the same sublattice} \\ -1 & \text{i , j are on the different sublattice} \end{cases}$$

MEASUREMENT OF D(R) --- TRANSITION GRAPH

Four Spin Correlation D(r)



$$\frac{\langle V_\beta|(\mathbf{S}_k\cdot\mathbf{S}_l)(\mathbf{S}_i\cdot\mathbf{S}_j)|V_\alpha\rangle}{\langle V_\beta|V_\alpha\rangle} = \begin{cases} (\frac{9}{16}-\frac{3}{4}\delta^{ij}_{kl})\phi_{ij}\phi_{kl}, & (i,j,k,l)_L, \\ \frac{9}{16}\phi_{ij}\phi_{kl}, & (i,j)_L(k,l)_L, \\ \frac{3}{16}\phi_{ij}\phi_{kl}, & (i,k)_L(j,l)_L, \\ \frac{3}{16}\phi_{ij}\phi_{kl}, & (i,l)_L(j,k)_L. \end{cases}$$

$$\phi_{ij} = \begin{cases} +1 & \text{i , j are on the same sublattice} \\ -1 & \text{i , j are on the different sublattice} \end{cases}$$

$$\delta^{kl}_{ij} = \begin{cases} 1 & \text{k,l are in the same (i j) sub-loop} \\ 0 & \text{k,l are in different (i j) sub-loop} \end{cases}$$

YT, Anders W. Sandvik, and Christopher L. Henley Phys. Rev. B 84, 174427 (2011)
Kevin. S. D. Beach and Anders. W. Sandvik, Nuclear Physics B 750, 142 (2006)

MEASUREMENT OF C(R)

TASK TO DO

- Measure **C(r)** along y=1 axis in 1D, 2-leg ladder and 2D
- What forms do you get for C(r) in these 3 cases respectively?
- Compare results with available results obtained yesterday from SSE.
- Are they expected?

MEASUREMENT OF C(R)