Quantum Monte Carlo Methods at Work for Novel Phases of Matter

SSE TUTORIAL II (CONTINUED...)

Projector QMC for JQ_3 chain

Ying Tang

Anders Sandvik

Trieste , Italy 31/01/2012

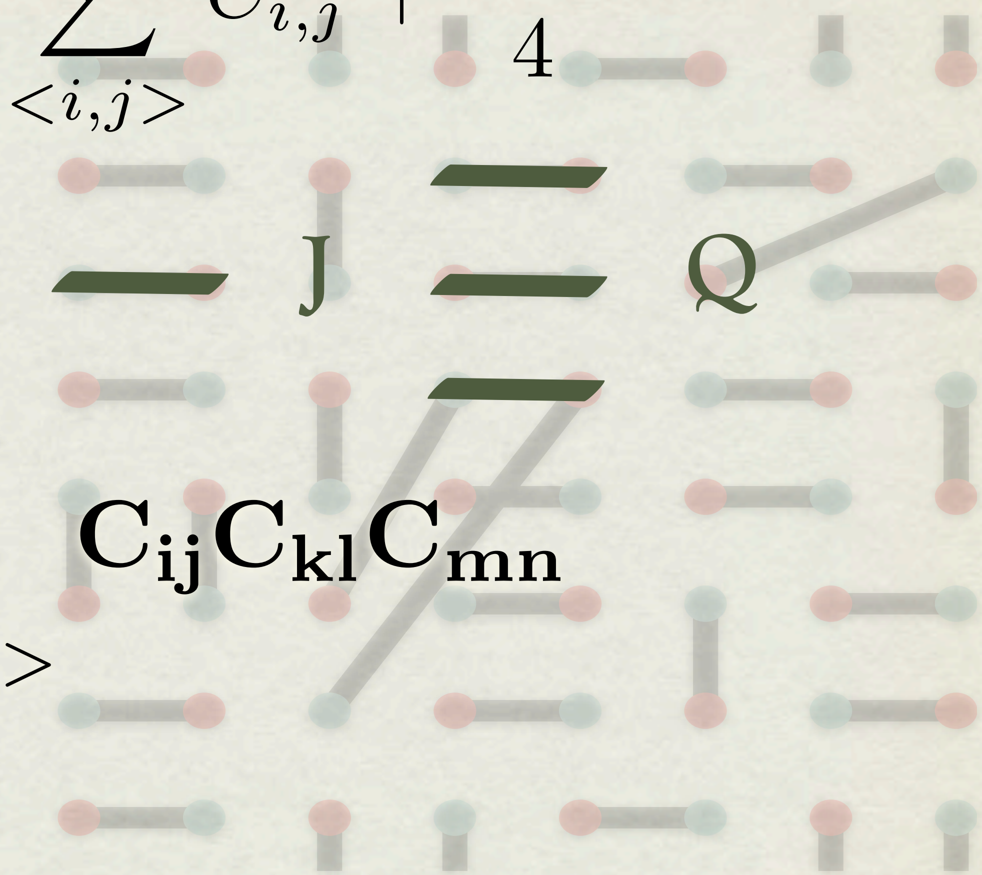
BOSTON UNIVERSITY

GO BEYOND HEISENBERG MODEL

- **Heisenberg Model**

$$C_{i,j} = \frac{1}{4} - \mathbf{S_i} \cdot \mathbf{S_j} \qquad H = -J \sum_{<i,j>} C_{i,j} + \frac{NJ}{4}$$

- **JQ$_3$ Model**



$$H = -J \sum_{<ij>} \mathbf{C_{ij}} - Q \sum_{<ijklmn>} \mathbf{C_{ij}C_{kl}C_{mn}}$$

Critical

Deep VBS

g_c=0.1645

VBS

g=Q/J

GO BEYOND HEISENBERG MODEL

- **Heisenberg Model**

$$H = -J \sum_{<i,j>} C_{i,j} + \frac{NJ}{4}$$

singlet projector operator

$$C_{i,j} = \frac{1}{4} - \mathbf{S_i} \cdot \mathbf{S_j} \qquad C_{i,j} = C^1_{i,j} + C^2_{i,j}$$

$$C^1_{i,j} = \frac{1}{4} - S^z_i S^z_j$$

diagonal operator

$$C^2_{i,j} = \frac{1}{2}(S^+_i S^-_j + S^-_i S^+_j)$$

off-diagonal operator

$$(-H)^m = \sum_{\{\alpha, a=1,2\}} \prod_{l=1}^{m} C^a_{i^\alpha_l j^\alpha_l} = \sum_{\{\alpha\}} P_{\{\alpha\}}$$

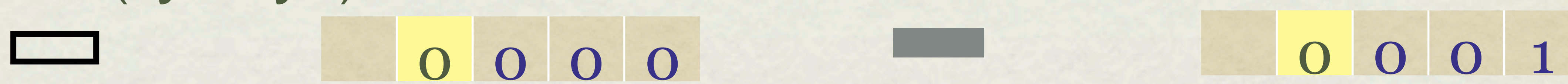
→ a string of operator $C_{i,j}$

GO BEYOND HEISENBERG MODEL

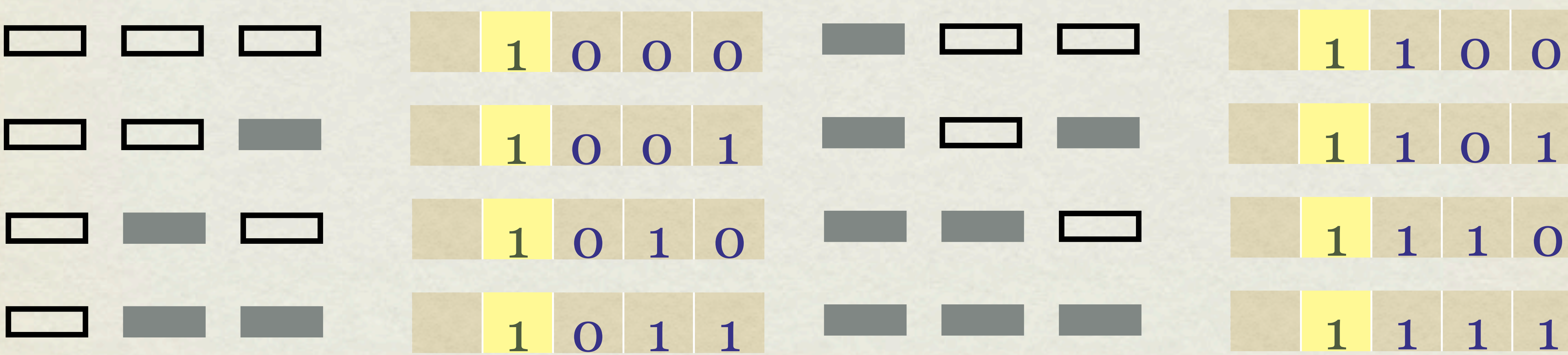
- **JQ3 Model**

$$H = -J \sum_{<ij>} \mathbf{C_{ij}} - Q \sum_{<ijklmn>} \mathbf{C_{ij}C_{kl}C_{mn}}$$

J Operator (<J> = J/2)



Q Operator (<Q> = Q/8)



$$(-H)^m = \sum_{\{\alpha,a\}} \prod_{l=1}^{m} \hat{O}^{a}_{i^\alpha_l j^\alpha_l} = \sum_{\{\alpha\}} P_{\{\alpha\}}$$

GET STARTED

- Download program to JQChain directory (e.g.~/JQChain)
- Generate input file **read.in** and random number seed file **seed.in** in the same directory.
- Compile program with **g95/gfortran**
    - **gfortran -O jq3chain.f90**
- run **./a.out**

read.in

```
nn, jj, qq, mm
init, nbins, mstps, istps
```

seed.in

```
an integer
```

```
nn     : chain length
jj, qq : J and Q values
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)
```

TASK TO DO-- OBSERVE VBS ORDER

Dimer Correlation D(r)

$$\frac{\langle V_\beta|(\mathbf{S}_k\cdot\mathbf{S}_l)(\mathbf{S}_i\cdot\mathbf{S}_j)|V_\alpha\rangle}{\langle V_\beta|V_\alpha\rangle}$$

$$= \begin{cases} \frac{9}{16} - \frac{3}{4}\delta^{ij}_{kl})\phi_{ij}\phi_{kl}, & (i,j,k,l)_L, \\ \frac{9}{16}\phi_{ij}\phi_{kl}, & (i,j)_L(k,l)_L, \\ \frac{3}{16}\phi_{ij}\phi_{kl}, & (i,k)_L(j,l)_L, \\ \frac{3}{16}\phi_{ij}\phi_{kl}, & (i,l)_L(j,k)_L. \end{cases}$$

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

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

read.in

```
32, 0, 1, power
0, 10, 10000, 10000
```

takes 36 seconds on mac air

read.in

```
32, 1, 0, power
0, 10, 10000, 10000
```

takes 20 seconds on mac air

a.out --> cor.dat

(r, C(r), D(r))

b.out --> c.dat

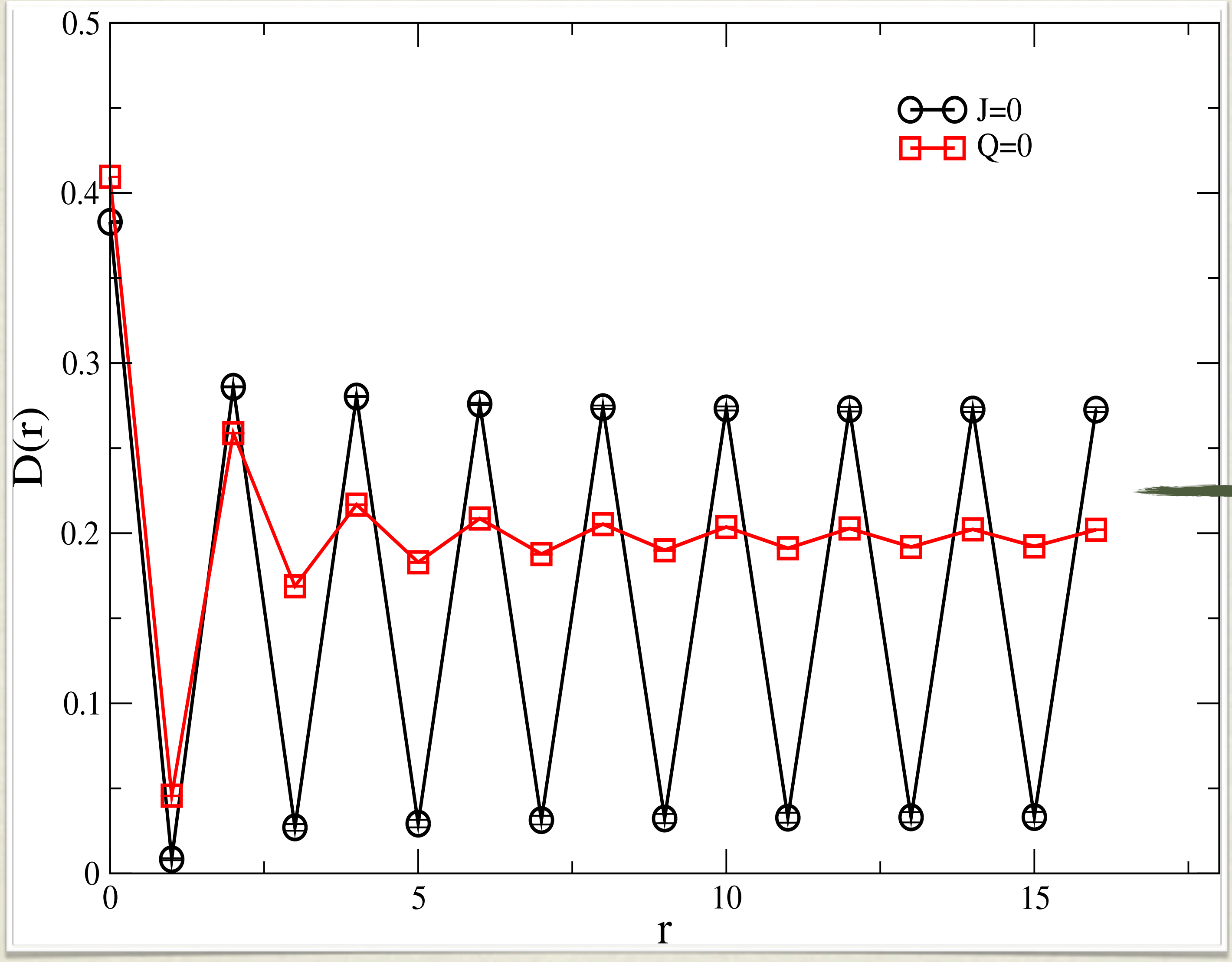
(C(r), D(r) and D*(r) w/ error bars)

TASK TO DO-- OBSERVE VBS ORDER

What do you observe if you plot D(r) versus r ?

TASK TO DO-- OBSERVE VBS ORDER

What do you observe if you plot D(r) versus r ?



Staggered Pattern

TASK TO DO-- OBSERVE VBS ORDER

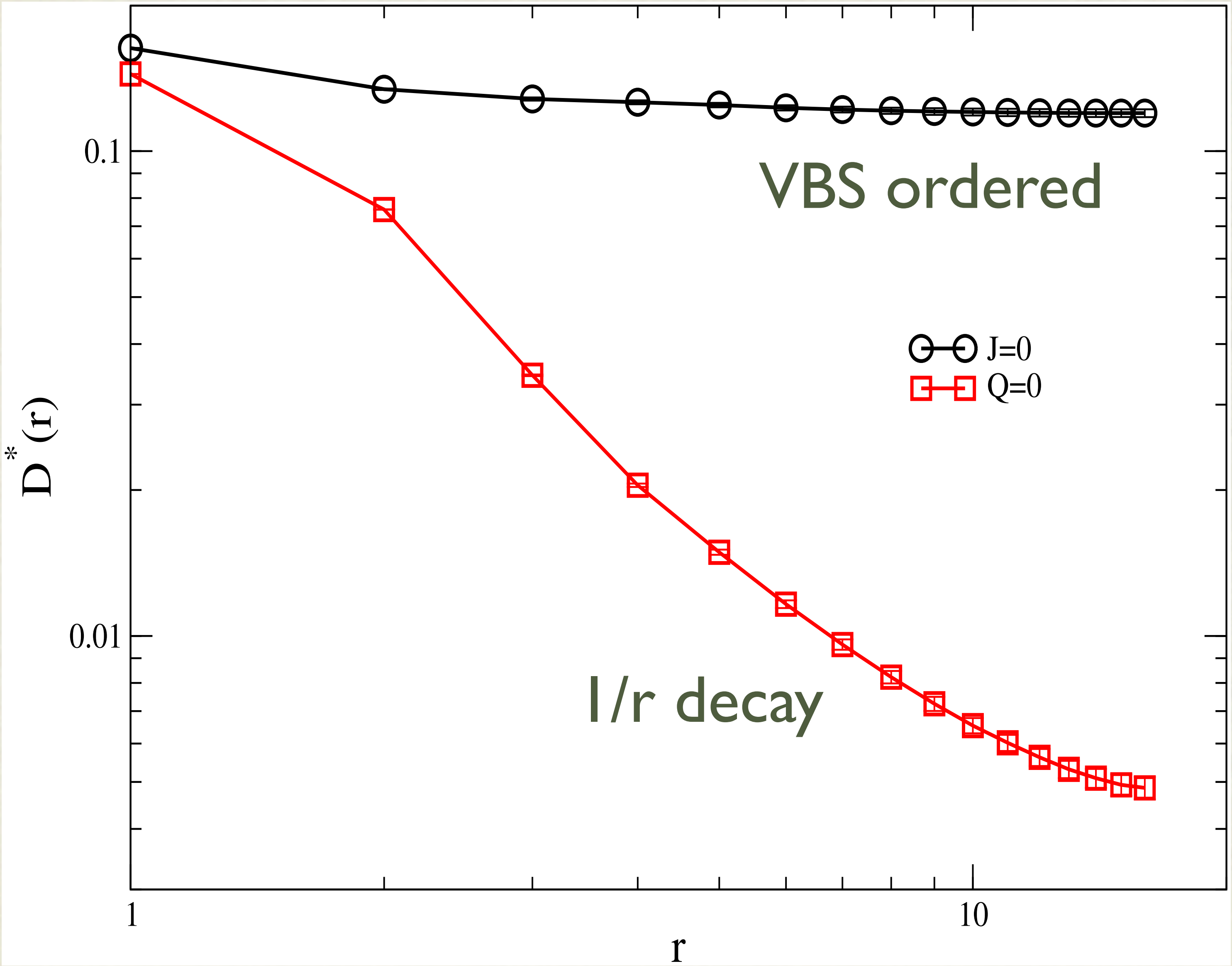
$D^*(r)=\{D(r)-1/2[D(r-1)+D(r+1)]\}^*(-1)^r$

↘

Subtract Staggered part

TASK TO DO-- OBSERVE VBS ORDER

$D^*(r)=\{D(r)-1/2[D(r-1)+D(r+1)]\}^*(-1)^r$



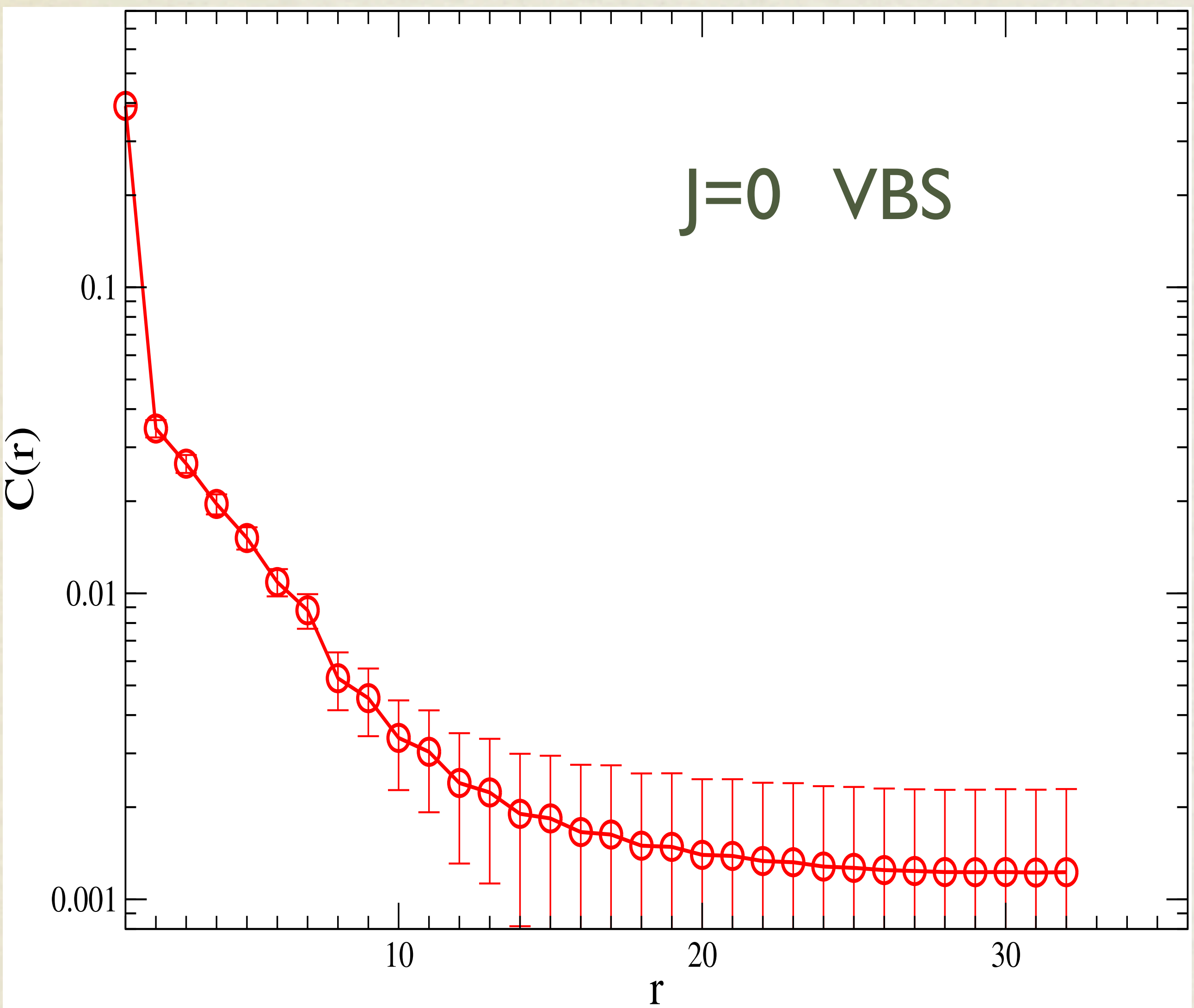
Subtract Staggered part

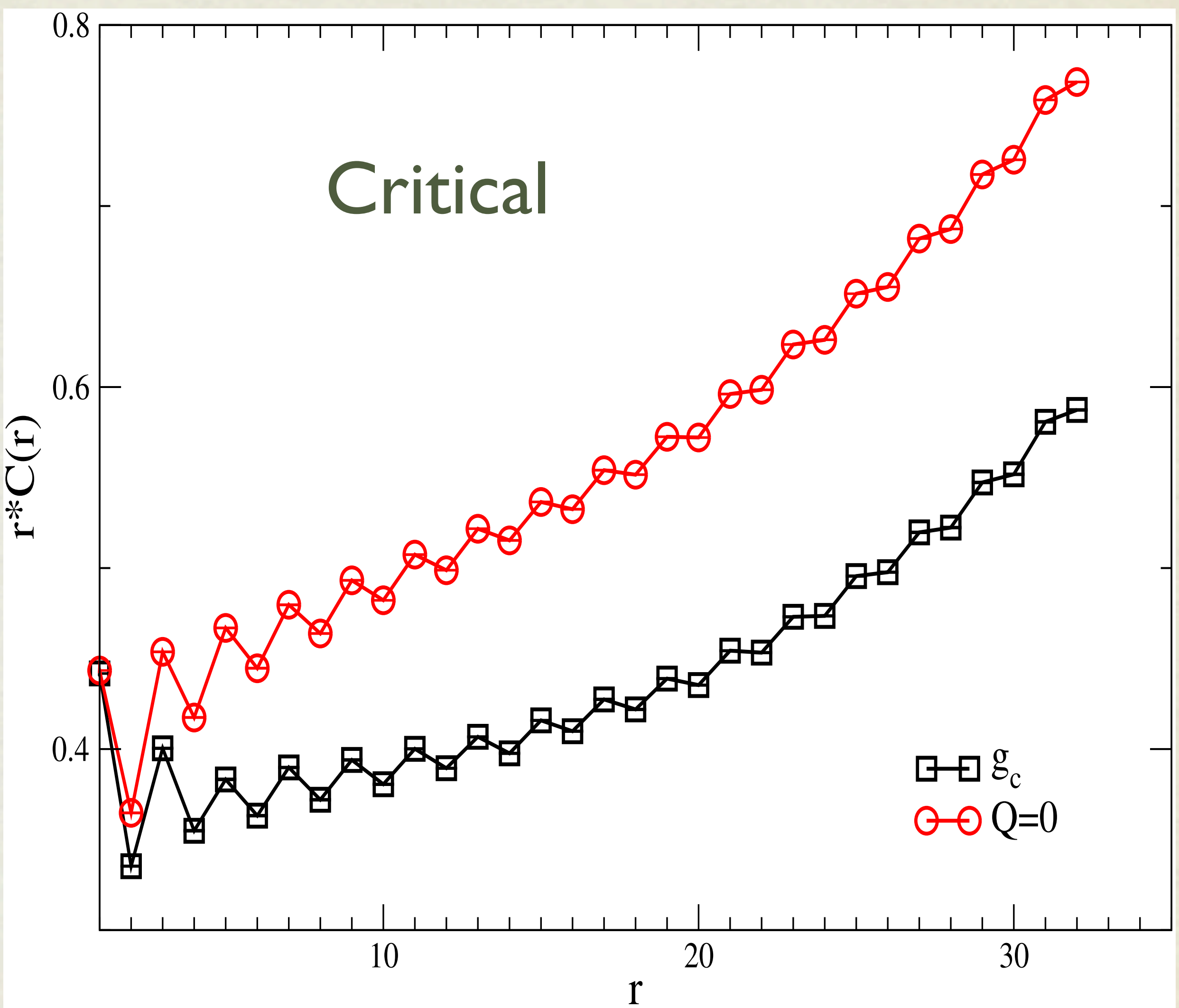
OBSERVE VBS ORDER

TASKS TO DO

- Measure **C(r), D*(r)** with **L=64** (~4 mins) or **larger** system with different **Q/J** ratios.
- What forms do you get for **C(r)** and **D(r)**, at different **Q/J** (0, >>1, and 0.1645)?
- **Explanations**?

TASK TO DO-- OBSERVE VBS ORDER C(R)





TASK TO DO-- OBSERVE VBS ORDER D*(R)