SSE TUTORIAL II

Projector QMC for Heisenberg model

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Trieste, Italy    31/01/2012
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)
The program can be found at:

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

Heisenberg Model

\[ H = \sum_{<i,j>} J \mathbf{S}_i \cdot \mathbf{S}_j \]
\[ \langle A \rangle = \frac{\langle \psi_1 | (-H)^m A (-H)^m | \psi_2 \rangle}{\langle \psi_1 | (-H)^{2m} | \psi_2 \rangle} \]

\[ \langle V'_\beta | V'_\alpha \rangle \]

Power m should be large enough to obtain ground states.
\( |V_\beta\rangle \)
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, msteps, isteps | 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

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

```
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
... ...
```

- **Output files:**
  - `cor.dat`  
    - [ r and C(r)]
  - `c.dat`  
    - `error`

Note, real power = 64*N/2

(takes ~14 seconds on macbook air)
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

<table>
<thead>
<tr>
<th>Parameter</th>
<th>SSEbasic</th>
<th>PMCbasic</th>
</tr>
</thead>
<tbody>
<tr>
<td>$3C^z(L/2)$</td>
<td>0.04550466</td>
<td>0.00036189</td>
</tr>
<tr>
<td>$C(L/2)$</td>
<td>0.04552031</td>
<td>0.00010459</td>
</tr>
</tbody>
</table>

Suggested Parameters (challenge large L)
- $L=32$
- $\beta=64$ (sse)
- $mm=64$ (projector)
- $bin=10$, $mcstep=1000$

TASK TO DO

- Compare $(mc=10^5, \sim 30$ mins)
TEST OF CONVERGENCE

TASK TO DO

- At a fixed r (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:

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

singlet gap $\Delta \propto 1/L$

1D Chain, L=32, bin=10, mstps=10^4
(takes a couple of minutes)

answer: $m \sim NL$
MEASUREMENT OF $C(r)$ --- TRANSITION GRAPH

\[ C(r_{ij}) = \frac{\langle V_\beta | S_i \cdot S_j | V_\alpha \rangle}{\langle V_\beta | V_\alpha \rangle} \]

\[ = \begin{cases} 
0, & (i)_L (j)_L \\
\frac{3}{4} \phi_{ij}, & (i, j)_L 
\end{cases} \]

\[ \phi_{ij} = \begin{cases} 
+1, & i, j \text{ are on the same sublattice} \\
-1, & i, j \text{ are on the different sublattice} 
\end{cases} \]
Four Spin Correlation $D(r)$

\[
\frac{\langle V_\beta | (S_k \cdot S_l)(S_i \cdot S_j) | V_\alpha \rangle}{\langle V_\beta | V_\alpha \rangle} = \begin{cases} 
\left(\frac{9}{16} - \frac{3}{4} \delta^{ij}_{kl}\right) \phi_{ij} \phi_{kl}, & (i,j,k,l) \_ L \\
\frac{9}{16} \phi_{ij} \phi_{kl}, & (i,j) \_ L (k,l) \_ L \\
\frac{3}{16} \phi_{ij} \phi_{kl}, & (i,k) \_ L (j,l) \_ L \\
\frac{3}{16} \phi_{ij} \phi_{kl}, & (i,l) \_ L (j,k) \_ L .
\end{cases}
\]

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

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