Quantum Monte Carlo Methods at Work for Novel Phases of Matter

SSE TUTORIAL I

SSE for Heisenberg model

Ying Tang
Anders Sandvik

Trieste 30/01/2012
Tour inside ssebasic.f90
Test convergence of the program
Test correction of the program
Finite size scaling of sublattice magnetization
Write your own measurement of spin-spin correlation (z component only)
- The program can be found at:

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

- Heisenberg Model

\[ H = \sum_{\langle i,j \rangle} J \mathbf{S}_i \cdot \mathbf{S}_j \]
GET STARTED

- Download it to a SSE directory (e.g. ~/SSE)

- Generate input file `read.in` and random number seed file `seed.in` in the same directory.

- Compile program with `g95/gfortran`
  ```
gfortran -O ssebasic.f90
  ```

- run `./a.out`  
  `lx` and `ly` should be even or `ly=1`

read.in

<table>
<thead>
<tr>
<th>lx, ly, beta</th>
</tr>
</thead>
<tbody>
<tr>
<td>nbins, msteps, isteps</td>
</tr>
</tbody>
</table>

seed.in

| an integer |

lx, ly : lattice size in x and y direction  
beta : inverse dimensionless temperature J/T  
nbins : Number of bins (averages written to file 'res.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)
### AN EXAMPLE

#### read.in

8 8 2
10 10000 10000

(takes a few seconds on macbook air)

#### res.dat

<table>
<thead>
<tr>
<th>energy</th>
<th>specific heat</th>
<th>sublattice (&lt;m^2&gt;)</th>
<th>susceptibility</th>
</tr>
</thead>
<tbody>
<tr>
<td>-0.60545312499999993</td>
<td>0.456631187500002241</td>
<td>0.1293503187647464</td>
<td>7.49062499999999937E-002</td>
</tr>
<tr>
<td>-0.60682343749999990</td>
<td>0.44244269437507455</td>
<td>0.12865359015698782</td>
<td>7.48968750000000016E-002</td>
</tr>
<tr>
<td>-0.60736640624999993</td>
<td>0.42738905609377298</td>
<td>0.12857748019236501</td>
<td>7.65843749999999962E-002</td>
</tr>
<tr>
<td>-0.60639140624999999</td>
<td>0.47596175609373859</td>
<td>0.13036687638192762</td>
<td>7.63156249999999984E-002</td>
</tr>
<tr>
<td>-0.60511015625000009</td>
<td>0.39663114359370866</td>
<td>0.12531685491597871</td>
<td>7.72593750000000051E-002</td>
</tr>
<tr>
<td>-0.60642031250000006</td>
<td>0.42985882437494638</td>
<td>0.13028933087043010</td>
<td>7.49156249999999996E-002</td>
</tr>
<tr>
<td>-0.60657500000000009</td>
<td>0.52802733499999337</td>
<td>0.13139164458652658</td>
<td>7.49156249999999996E-002</td>
</tr>
<tr>
<td>-0.60642031250000006</td>
<td>0.42871590234381074</td>
<td>0.1319164458652658</td>
<td>7.49156249999999996E-002</td>
</tr>
<tr>
<td>-0.60733203124999990</td>
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<td>0.12873853782797756</td>
<td>7.72593750000000051E-002</td>
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<tr>
<td>-0.60511015625000009</td>
<td>0.53154232437492510</td>
<td>0.12912797510686908</td>
<td>7.72593750000000051E-002</td>
</tr>
</tbody>
</table>
**AN EXAMPLE**

<table>
<thead>
<tr>
<th>energy &lt;e&gt;</th>
<th>specific heat &lt;c&gt;</th>
<th>sublattice &lt;m²&gt;</th>
<th>susceptibility χ</th>
</tr>
</thead>
<tbody>
<tr>
<td>-0.60545312499999993</td>
<td>0.45663118750002241</td>
<td>0.12939503187647464</td>
<td>7.49062499999999937E-002</td>
</tr>
<tr>
<td>-0.60682343749999990</td>
<td>0.44244269437507455</td>
<td>0.12865359015698782</td>
<td>7.48968750000000016E-002</td>
</tr>
<tr>
<td>-0.60736640624999993</td>
<td>0.47596175609373859</td>
<td>0.12857748019236501</td>
<td>7.65843749999999996E-002</td>
</tr>
<tr>
<td>-0.60639140624999999</td>
<td>0.42985882437494638</td>
<td>0.13036687638192762</td>
<td>7.74468749999999984E-002</td>
</tr>
<tr>
<td>-0.60511015625000009</td>
<td>0.52802733499993337</td>
<td>0.13251685491597871</td>
<td>7.49156249999999996E-002</td>
</tr>
<tr>
<td>-0.60642031250000006</td>
<td>0.42871590234381074</td>
<td>0.13185469109301354</td>
<td>7.72593750000000051E-002</td>
</tr>
<tr>
<td>-0.60733203124999990</td>
<td>0.53947162249994562</td>
<td>0.13185469109301354</td>
<td>7.72593750000000051E-002</td>
</tr>
<tr>
<td>-0.60921562500000004</td>
<td>0.53154232437492510</td>
<td>0.13185469109301354</td>
<td>7.72593750000000051E-002</td>
</tr>
</tbody>
</table>

**res.dat**

```
res.dat
```

- Compile error bars
  - compile res.f90
  ```
gfortran -o b.out -O res.f90
  ```
- Run ./b.out
  ```
run ./b.out
  ```

<table>
<thead>
<tr>
<th>e.dat</th>
<th>m.dat</th>
</tr>
</thead>
<tbody>
<tr>
<td>&lt;e&gt;</td>
<td>&lt;m²&gt;</td>
</tr>
<tr>
<td>-0.60694234</td>
<td>0.12937120</td>
</tr>
<tr>
<td>e error</td>
<td>m² error</td>
</tr>
<tr>
<td>0.00040847</td>
<td>0.00057857</td>
</tr>
<tr>
<td>&lt;c&gt;</td>
<td>&lt;χ&gt;</td>
</tr>
<tr>
<td>0.46566718</td>
<td>0.07635813</td>
</tr>
<tr>
<td>c error</td>
<td>χ error</td>
</tr>
<tr>
<td>0.01608355</td>
<td>0.00034245</td>
</tr>
</tbody>
</table>
We also have to modify the stored spin state after the loop update:

- we can use the information in $V_{\text{first}}$ and $X()$ to determine spins to be flipped.
- Spins with no operators, $V_{\text{first}}(i) = 1$, flipped with probability $1/2$.

```plaintext
do i = 1 to N
  v = V_{\text{first}}(i)
  if (v = 1) then
    if (random[0-1] < 1/2) then
      i = i
    else
      if (X(v) = 2) then
        i = i
  endif
enddo
```

$v$ is the location of the first vertex leg on spin $i$:
- Flip it if $X(v) = 2$.
- (Do not flip it if $X(v) = 1$).
- No operation on $i$ if $V_{\text{first}}(i) = 1$.

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**Determination of the cut-off $L$**

- Adjust during equilibration.
- Start with arbitrary (small) $n$.
- Keep track of number of operators $n$.
- Increase $L$ if $n$ is close to current $L$.
- E.g., $L = n + n/3$.

**Example:** 16"16 system, $L = 16$.

**Evolution of $L$**

**$n$ distribution after equilibration**

**Truncation is no approximation.**

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In this program, we only record $L$ values once there is an increment.
TEST OF CORRECTNESS
CHECK THE GROUND STATE ENERGY OF HEISENBERG CHAIN

Lx=32, Ly=1 20 bins and 10,000 MC steps, use large $\beta$

<table>
<thead>
<tr>
<th>beta</th>
<th>$\langle e \rangle$</th>
<th>error</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.0</td>
<td>-0.20477922</td>
<td>0.00016893</td>
</tr>
<tr>
<td>2.0</td>
<td>-0.34135748</td>
<td>0.00016988</td>
</tr>
<tr>
<td>4.0</td>
<td>-0.41897368</td>
<td>0.00007303</td>
</tr>
<tr>
<td>8.0</td>
<td>-0.43776850</td>
<td>0.00003716</td>
</tr>
<tr>
<td>16.0</td>
<td>-0.44240240</td>
<td>0.00002830</td>
</tr>
<tr>
<td>32.0</td>
<td>-0.44377160</td>
<td>0.00002360</td>
</tr>
<tr>
<td>64.0</td>
<td>-0.44394747</td>
<td>0.00002178</td>
</tr>
</tbody>
</table>

exact $e$: -0.44395398

about 10 mins on macbook air
FINITE SIZE SCALING OF $M_s^2$

\[ < m_s > = \frac{1}{N} \sum_{i=1}^{N} \phi_i S_i \quad < m_s^2 > = \frac{1}{N^2} \sum_{i,j=1}^{N} \phi_i \phi_j S_i S_j = \frac{1}{N} \int C(r) dr \]

\[ C(r) = < S_i \cdot S_{i+r} > \]

**TASK TO DO**

- run 1D, 2-leg ladder and 2D program for several sizes $L_x$
- Plot $L_x < m_s^2 >$ vs $L_x$ for 1D and Ladder
- Plot $< m_s^2 >$ vs $1/L_x$ for 2D

*Suggested Parameters (takes a few minutes)*

1D: $\beta=2L$, $L=8$, 16, 32, 64
2-Leg Ladder: $\beta=64$, $L=8$, 16, 32
2D ($N=L^2$): $\beta=2L$, $L=4$ to 16
$\text{bin}=10 \quad \text{mc step}=10,000$

Do more data points if time allows!

*Questions to think about:*

Why do we multiply 1D and Ladder $< m_s^2 >$ with $L_x$ while plot 2D $< m_s^2 >$ versus inverse $L_x$? (key: $C(r)$)

Why do we increase $\beta$ as a function of system size in 1D and 2D Heisenberg Model? Why do you keep $\beta$ as constant in 2-leg ladder? (key: gap)
FINITE SIZE SCALING OF $M_S^2$

Can be explained by:

$$<m_s^2> = \frac{1}{N} \int C(r) dr$$
MEASUREMENT OF \( C^z(R) \)

\[
C^z(r) = \langle S^z_i \cdot S^z_{i+r} \rangle
\]

**TASK TO DO**

- Add a simple subroutine to measure \( z \) component of spin-spin correlation \( C^z(r) \) for 1D, 2-leg Ladder and 2D systems (only along \( y=1 \) for 2-leg ladder and 2D systems).

- Modify res.f90 to calculate error bars for \( C^z(r) \).

- Plot \( C^z(r) \) versus \( L_x \). What forms do you get? Are they expected?

1st step -> create an array in measurementdata module:

\[
\text{real}(8), \text{allocatable} :: \text{crr}(:) \]

Do the measurement in the subroutine **measure**
MEASUREMENT OF $C^Z(r)$

Graphs showing the measurement of $C^Z(r)$ for different values of $L$: $L=32$ for ladder and $L=24$ for 2D.
FINITE SIZE SCALING OF $M_S^2$

\[ \langle m_s^2 \rangle = \frac{1}{N} \int C(r) dr \]

$r \gg 1$

1D \quad \quad C(r) \propto \frac{1}{r}

Ladder \quad \quad C(r) \propto e^{-\frac{r}{\xi}}

2D \quad \quad \text{constant}
real(8), allocatable :: crr(:)
allocate(crr(0:nn/2)) !allocate spin-spin correlator

do s1=1, nn  ! nn: spin number
   x=mod(s1-1,lx)  !x index
   y=int((s1-1)/lx) !y index
   do r=0, lx/2
      s2=mod(x+r,lx)+y*lx+1
      crr(r)=crr(r)+spin(s1)*spin(s2)
   end do
end do

crr=0.25d0*crr/dble(nn)/dble(msteps)
deallocate(crr)