# P452 TERM PAPER:Monte carlo Simulation for 1-D spin 1/2 chain.

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**Abstract**

This is a report on monte-carlo simulation of 1-D spin 1/2 fermionic lattice chain for the course P452 semester 8.

I took finite 1-D chains of spin 1/2.My aim was to calculate expectation value of nearest neighbour spin correlation with half filled states.The simulation showed that spin correlation varies roughly as $1/N^2$ where N is the number of lattice sites.With large N limit , the spin correlation value agrees moderately with analytic results.

## 1 Theory:

**Hubbard Model:**

$$\mathcal{H} = -t \sum_{<ij>} \sum_{\sigma} (C^{\dagger}_{i\sigma} C_{j\sigma} + h.c) + U \sum_{i} n_{i\uparrow} n_{i\downarrow} \quad (1)$$

Where $C^{\dagger}_{i\sigma}$ creates electron of spin $\sigma$ at site i.The fermionic operators obeys the anti commutation relations.

The spin-1/2 operator at site i is given as:

$$\mathbf{S_i} = \frac{1}{2} \sum_{\alpha,\beta} C^{\dagger}_{i\sigma} \sigma_{\alpha\beta} C_{i\sigma}$$

where $\sigma_{\alpha\beta}$ are the components of vector $\sigma$ of Pauli matrices.

The exactly half filled band case is characterized by a ground state with one electron per site i.e there are no empty sites or holes.The effective Hamiltonian becomes a pure antiferromagnetic Heisenberg Hamiltonian[1]:

$$\mathcal{H} = J \sum_{<ij>} \mathbf{S_i}.\mathbf{S_j} \quad (2)$$

Where J:=J(t,U)>0.

A popular variational state for monte-carlo calculations is Gutzwiller wave function.

$$|\psi\rangle = \Pi_j [1 - (1-g) n_{j\uparrow} n_{j\downarrow}] |\phi\rangle \quad (3)$$

Where $|\phi\rangle$is paramagnetic ground state of free electron which will be given by the slatter determinants.g is the variational parameter.$n_{j\uparrow}$and $n_{j\downarrow}$are the number operator.When g=0 ,we project out the states where there is no double occupancy.In my work I have taken g=0 and half filled states.Also I have taken equal number of up and down spins electrons.So if there are 2N lattice sites then there are N up spin and N down spin electrons.

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The amplitude of particular configuration is given by the slatter determinant can be realized in the following steps:

$$|\phi\rangle = (C^{\dagger}_{k_1\uparrow} C^{\dagger}_{K_2\uparrow} ..... C^{\dagger}_{K_{N/2}\uparrow}).(C^{\dagger}_{k_1\downarrow} C^{\dagger}_{K_2\downarrow} ..... C^{\dagger}_{K_{N/2}\downarrow}) |0\rangle$$

Where $C^{\dagger}_{k_i\sigma}$ creates a electron of spin sigma of momentum $k_i$.Now we do fourier transformation to real space.

$$C^{\dagger}_{k_i\sigma} = \sum_{r_j} e^{ik_i.r_j} C^{\dagger}_{r_j\sigma}$$

$$|\phi\rangle = (\sum_{r_j} e^{ik_1.r_j} C^{\dagger}_{r_j\uparrow})(\sum_{r_j} e^{ik_2.r_j} C^{\dagger}_{r_j\uparrow}).....(\sum_{r_j} e^{ik_{N/2}.r_j} C^{\dagger}_{r_j\uparrow}).$$
$$(\sum_{r_j} e^{ik_1.r_j} C^{\dagger}_{r_j\downarrow})(\sum_{r_j} e^{ik_2.r_j} C^{\dagger}_{r_j\downarrow}).....(\sum_{r_j} e^{ik_{N/2}.r_j} C^{\dagger}_{r_j\downarrow}) |0\rangle$$

[1]Modles of Quantum Matter:Hans-Peter Eckle

$$= \sum (e^{ik_1.r_{j1}} e^{ik_2.r_{j2}} ... e^{ik_{N/2}.r_{j_{N/2}}}).(e^{ik_1.r_{l1}} e^{ik_2.r_{l2}} ... e^{ik_{N/2}.r_{l_{N/2}}}) \times$$
$$C^{\dagger}_{r_{j1}\uparrow} C^{\dagger}_{r_{j2}\uparrow} ... C^{\dagger}_{r_{j_{N/2}}\uparrow} . C^{\dagger}_{r_{l1}\downarrow} C^{\dagger}_{r_{l2}\downarrow} ... C^{\dagger}_{r_{l_{N/2}}\downarrow} |0\rangle$$

For same configuration $\{r_{j1}, r_{j2}, .., r_{jN/2}\}$ the term $C^{\dagger}_{r_{j1}\uparrow} C^{\dagger}_{r_{j2}\uparrow} ... C^{\dagger}_{r_{j_{N/2}}\uparrow}$ can be written in all permutations,but since we are dealing with fermions ,anticommuataion relations of fermionic operators,sign changes will occur and the coffiecients will be given by slatter determinants.The cofficents will be product of two slatter determinants $D_{\uparrow}(k1, k2, ..kN/2, r_j1, rj2...rjN/2)$ and $D_{\downarrow}(k1, k2, ..kN/2, r_l1, rl2...rlN/2)$.

| No of Sites | $< S^z_i, S^z_{i+1} >$ | Std.Deviation | No of Sites | $< S^z_i, S^z_{i+1} >$ | Std.Deviation |
|---|---|---|---|---|---|
| 6 | -0.180132 | 0.083382 | 100 | -0.145435 | 0.019728 |
| 10 | -0.166549 | 0.062535 | 120 | -0.148888 | 0.018072 |
| 16 | -0.159069 | 0.04892 | 140 | -0.149527 | 0.016989 |
| 20 | -0.156749 | 0.043613 | 160 | -0.149427 | 0.016168 |
| 30 | -0.153282 | 0.03622 | 180 | -0.149214 | 0.015261 |
| 40 | -0.151247 | 0.030988 | 200 | -0.146603 | 0.014348 |
| 50 | -0.150736 | 0.02754 | 250 | -0.147912 | 0.014329 |
| 60 | -0.148652 | 0.025974 | 300 | -0.147677 | 0.012305 |
| 70 | -0.150651 | 0.023747 | 500 | -0.146321 | 0.009853 |
| 80 | -0.150164 | 0.022661 | 1000 | -0.144949 | 0.010102 |
| 90 | -0.150209 | 0.020918 | | | |

Table 1: Nearest neighbour Spin correlation vs number of sites.(Each evaluated with $10^6$ samples)

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The slatter determinant takes the form of vandermonde determinant.

$$\begin{vmatrix} 1 & z_1 & z_1^2 & ..... & z_1^{N_\sigma - 1} \\ 1 & z_2 & z_2^2 & ..... & z_2^{N_\sigma - 1} \\ 1 & z_3 & z_3^2 & ..... & z_3^{N_\sigma - 1} \\ . & & & ..... & \\ . & & & & \\ . & & & & \\ 1 & & & ..... & z_{N_\sigma}^{N_\sigma - 1} \end{vmatrix}$$

where $z_l = exp(i\Delta k r_l)$,$\Delta K = 2\pi/L$. This determinant is given by:

$$\prod_{l,m(l<m)} (z_l - z_m)$$

If we change the position of one electron then the ratio of two such determinants will be given by

$$\prod_{m(m\neq n)} \frac{(z_n - z_m)}{(z'_n - z_m)}$$

When the positions of only n'th electron has been changed from $r_n$ to $r'_n$.

$$|z_l - z_m|^2 = 4sin^2[\Delta k(\frac{r_i - r_m}{2})]$$

## 2 Algorithm:

1. Start with an initial state or configuration $\alpha$of spins.Calculate the spin correlation $S^z_i.S^z_{i+j}$.

2. Vary the configuration by exchanging positions of two electrons with opposite spins randomly to get new configuration $\alpha'$.Calculate the ratio of amplitudes $|\frac{p_\alpha}{p_{\alpha\prime}}|^2$.

3. Metropolis aceeptance :Accept or reject the new configuration with probability $\min(1,|\frac{p_\alpha}{p_{\alpha\prime}}|^2)$.

4. If accepted Calculate the spin correlation with this new configuration.

5. Do step 2 again to accumulate enough samples.

6. Compute average of spin correlation: $< S^z_i.S^z_{i+j} >$.

   There are huge number of possible configurations for even one dimensional chain.It is computationally intractable to compute the spin correlation for each configuration one by one as the chain size grows.Monte carlo method

provides feasible way to get an estimation on the expactation value of spin correlation.

## 3 Nearest neighbour spin correlation

The results are liste in table 1.The following are plots.The exact (Bethe-ansatz solution) result for the antiferromagnetic Heisenberg chain (AFH) is

$$q_1^{AFH} = -\frac{1}{3}(ln2 - \frac{1}{4}) = -0.1477157...$$

From linear fit my result is $q_1(\infty) = -0.150635 \pm 0.000893$.Also taking the linear fit range between 0 to 0.01 I got $q_1(\infty) = -0.149709 \pm 0.000665$

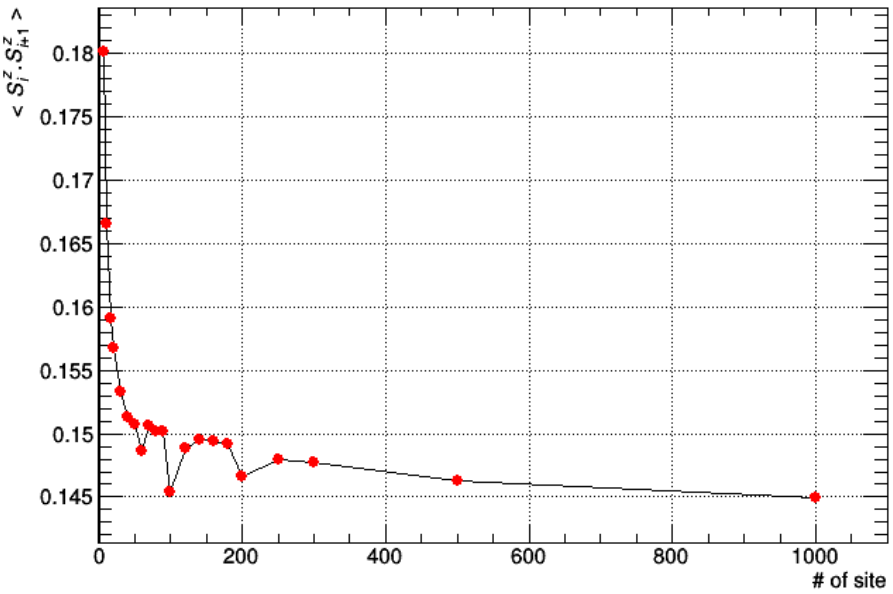


Figure 1: absolute value of spin correlation vs Number of sites

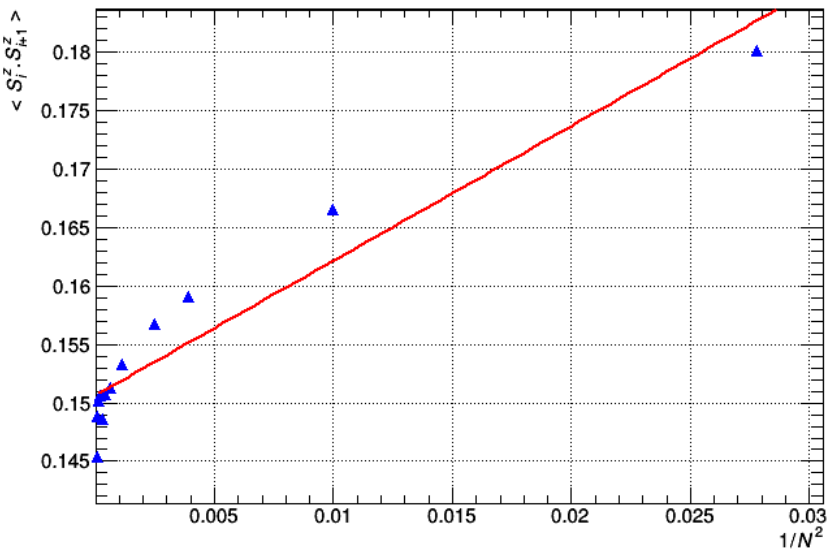


Figure 2: absolute value of spin correlation vs inverse square of Number of sites

## 4 NN spin correlation:

| No of Sites | $< S_i^z, S_{i+2}^z >$ | Std.Deviation |
|---|---|---|
| 10 | 0.037789 | 0.115327 |
| 20 | 0.047058 | 0.080047 |
| 50 | 0.052784 | 0.050098 |
| 80 | 0.054786 | 0.040612 |
| 100 | 0.056182 | 0.035453 |
| 150 | 0.057105 | 0.028487 |
| 200 | 0.057169 | 0.0253 |
| 300 | 0.052938 | 0.020219 |
| 500 | 0.055012 | 0.016972 |
| 800 | 0.048969 | 0.015327 |

Table 2: Next Nearest neighbour Spin correlation vs number of sites.(Each evaluated with $10^6$ samples)

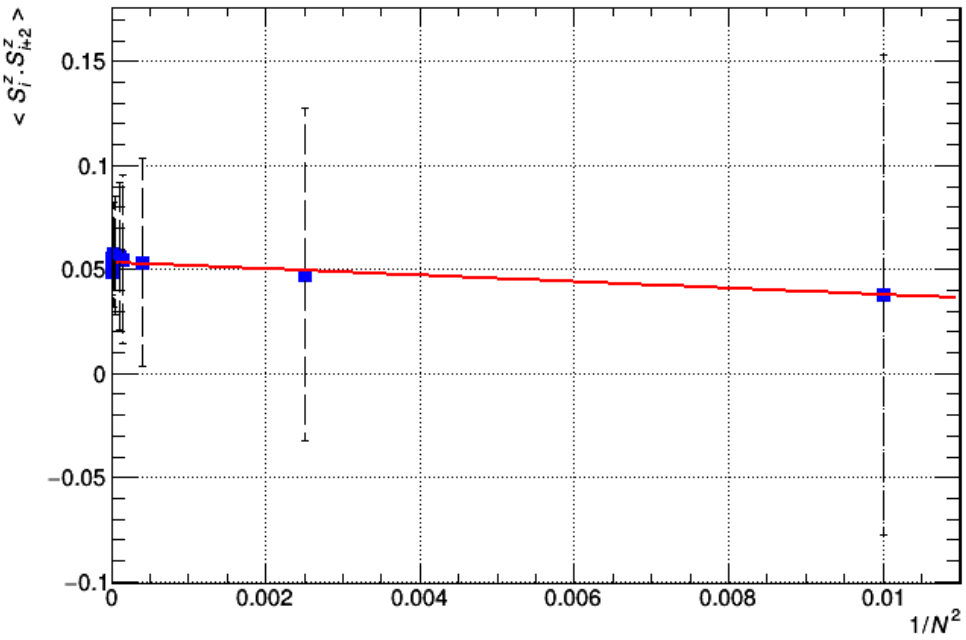


Figure 3: NN spin correlation vs inverse square of lattice sites.The error bars are very large compared to nearest neighbour spin correlation.

The extrapolated infinite limit NN spin correlation is: $q_2(\infty) = 0.0533536 \pm 0.008248$.

## 5 Discussion on results:

1. Since the Hamiltonian is rotation invariant(eq.2) we have $\mathbf{S}_i.\mathbf{S}_{i+1} = 3(S_i^z.S_{i+1}^z) = 0.0451905 \pm 0.002679$. This gives a estimation of ground state energy for half filled state(eq.2).
2. Figure 1 and 2 shows the $1/N^2$ dependence of spin correlation.
3. The standard deviation decreases with increase in number of lattice sites.Table 1.
4. The standard deviation in next nearest neighbour interaction is much greater than nearest neighbour interaction.

5. Nearest neighbour interaction spin correlation and next nearest neighbour spin correlation are opposite in sign ,so they are competing with each other.

6. The slope of linear fit in Next neighbour interaction is negative.This does not agree with previous works done in this topic[2].But Since The statistical error bars are very large(Fig .3)the confidence on the slope is very less.

# 6 References:


1. P Horsch and T A Kaplan 1983 J. Phys. C: Solid State Phys. 16 L1203

2. Antiferromagnetic correlations in almost-localized Fermi liquids.C. Gros, R. Joynt, and T. M. Rice,PHYSICAL REVIEW B VOLUME 36, NUMBER 1

3. Ceperley D M, Chester G V and Kalos M H 1977 Phys. Reo. B 16 3801

4. Gutzwiller M C 1963 Phys. Rev. Lett. 10 159


[2]P Horsch and T A Kaplan 1983 J. Phys. C: Solid State Phys. 16 L1203