

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:

Hamiltonian¹:

Hubbard Model:

$$\mathcal{H} = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j \quad (2)$$

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

Where $C_{i\sigma}^{\dagger}$ creates electron of spin σ at site i. The fermionic operators obey the anti commutation relations.

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

$$\mathbf{S}_i = \frac{1}{2} \sum_{\alpha, \beta} C_{i\alpha}^{\dagger} \boldsymbol{\sigma}_{\alpha\beta} C_{i\beta}$$

where $\sigma_{\alpha\beta}$ are the components of vector $\boldsymbol{\sigma}$ 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

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 Slater determinants. g is the variational parameter. $n_{j\uparrow}$ and $n_{j\downarrow}$ are the number operators. 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 spin electrons. So if there are $2N$ lattice sites then there are N up spin and N down spin electrons.

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

$$|\phi\rangle = (C_{k_1\uparrow}^{\dagger} C_{K_2\uparrow}^{\dagger} \dots C_{K_{N/2}\uparrow}^{\dagger}) \cdot (C_{k_1\downarrow}^{\dagger} C_{K_2\downarrow}^{\dagger} \dots C_{K_{N/2}\downarrow}^{\dagger}) |0\rangle$$

Where $C_{k_i\sigma}^{\dagger}$ creates an electron of spin sigma of momentum k_i . Now we do Fourier transformation to real space.

$$C_{k_i\sigma}^{\dagger} = \sum_{r_j} e^{ik_i \cdot r_j} C_{r_j\sigma}^{\dagger}$$

$$|\phi\rangle = \left(\sum_{r_j} e^{ik_1 \cdot r_j} C_{r_j\uparrow}^{\dagger} \right) \left(\sum_{r_j} e^{ik_2 \cdot r_j} C_{r_j\uparrow}^{\dagger} \right) \dots \left(\sum_{r_j} e^{ik_{N/2} \cdot r_j} C_{r_j\uparrow}^{\dagger} \right) \cdot \left(\sum_{r_j} e^{ik_1 \cdot r_j} C_{r_j\downarrow}^{\dagger} \right) \left(\sum_{r_j} e^{ik_2 \cdot r_j} C_{r_j\downarrow}^{\dagger} \right) \dots \left(\sum_{r_j} e^{ik_{N/2} \cdot r_j} C_{r_j\downarrow}^{\dagger} \right) |0\rangle$$

¹Modles of Quantum Matter: Hans-Peter Eckerle

$$= \sum (e^{ik_1.r_{j1}} e^{ik_2.r_{j2}} \dots e^{ik_{N/2}.r_{jN/2}}) \cdot (e^{ik_1.r_{l1}} e^{ik_2.r_{l2}} \dots e^{ik_{N/2}.r_{lN/2}}) \times \\ C_{r_{j1}\uparrow}^\dagger C_{r_{j2}\uparrow}^\dagger \dots C_{r_{jN/2}\uparrow}^\dagger \cdot C_{r_{l1}\downarrow}^\dagger C_{r_{l2}\downarrow}^\dagger \dots C_{r_{lN/2}\downarrow}^\dagger |0\rangle$$

For same configuration $\{r_{j1}, r_{j2}, \dots, r_{jN/2}\}$ the term $C_{r_{j1}\uparrow}^\dagger C_{r_{j2}\uparrow}^\dagger \dots C_{r_{jN/2}\uparrow}^\dagger$ can be written in all permutations, but since we are dealing with fermions, anticommutation relations of fermionic operators, sign changes will occur and the coefficients will be given by Slater determinants. The coefficients will be product of two Slater determinants $D_\uparrow(k_1, k_2, \dots, k_{N/2}, r_{j1}, r_{j2}, \dots, r_{jN/2})$ and $D_\downarrow(k_1, k_2, \dots, k_{N/2}, r_{l1}, r_{l2}, \dots, r_{lN/2})$.

No of Sites	$\langle S_i^z, S_{i+1}^z \rangle$	Std.Deviation	No of Sites	$\langle S_i^z, S_{i+1}^z \rangle$	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)

The Slater determinant takes the form of Vandermonde determinant.

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

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 .

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

2 Algorithm:

1. Start with an initial state or configuration α of spins. Calculate the spin correlation $S_i^z \cdot S_{i+j}^z$.
2. Vary the configuration by exchanging positions of two electrons with opposite spins randomly to get new configuration α' . Calculate the ratio of amplitudes $|\frac{p_\alpha}{p_{\alpha'}}|^2$.
3. Metropolis acceptance: Accept or reject the new configuration with probability $\min(1, |\frac{p_\alpha}{p_{\alpha'}}|^2)$.
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: $\langle S_i^z \cdot S_{i+j}^z \rangle$.

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 expectation value of spin correlation.

3 Nearest neighbour spin correlation

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

$$q_1^{AFH} = -\frac{1}{3}(\ln 2 - \frac{1}{4}) = -0.1477157...$$

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 $q_1(\infty) = -0.149709 \pm 0.000665$

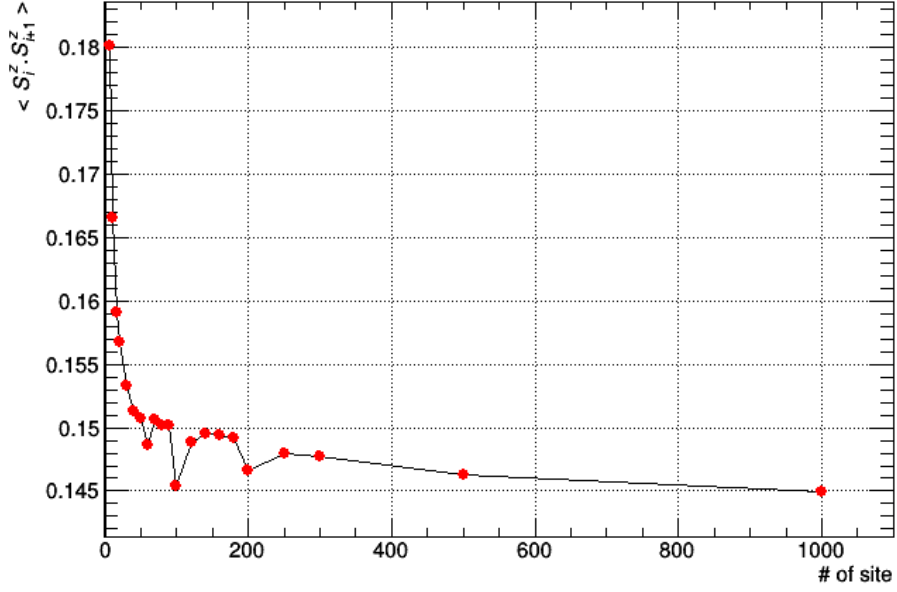


Figure 1: absolute value of spin correlation vs Number of sites

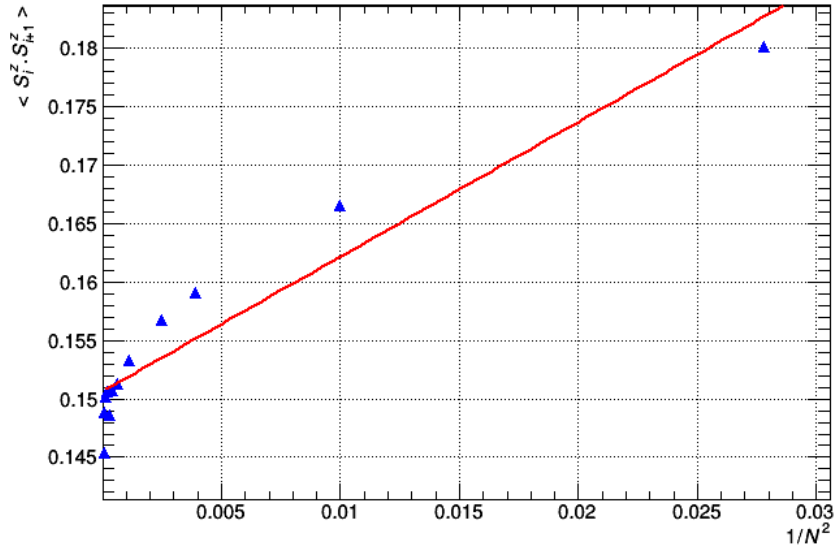


Figure 2: absolute value of spin correlation vs inverse square of Number of sites

4 NN spin correlation:

No of Sites	$\langle S_i^z, S_{i+2}^z \rangle$	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)

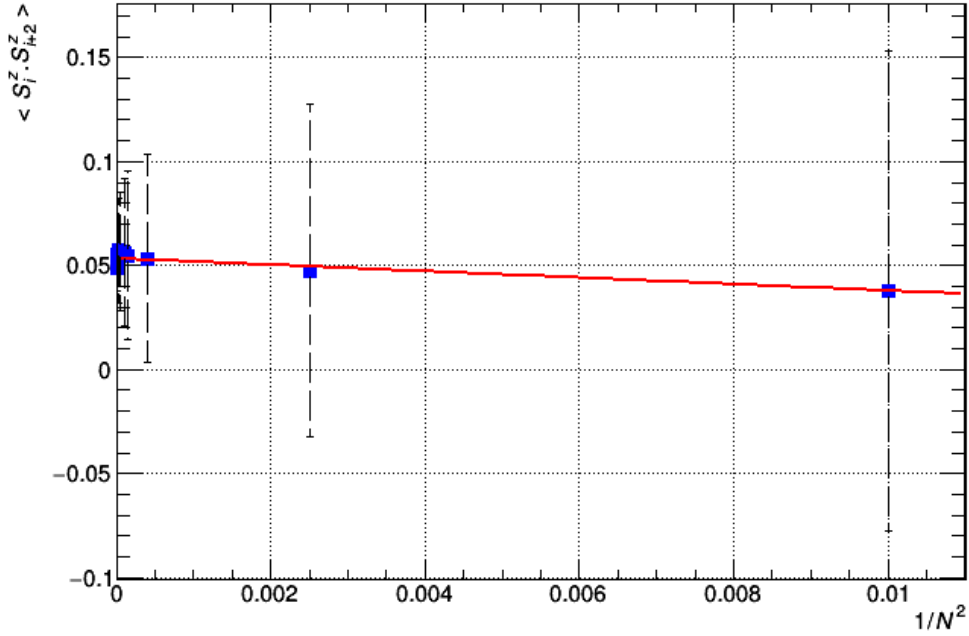


Figure 3: NN spin correlation vs inverse square of lattice sites. The error bars are very large compared to nearest neighbour spin correlation.

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 $\mathbf{S}_i \cdot \mathbf{S}_{i+1} = 3(S_i^z \cdot S_{i+1}^z) = 0.0451905 \pm 0.002679$. 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 topic².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

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