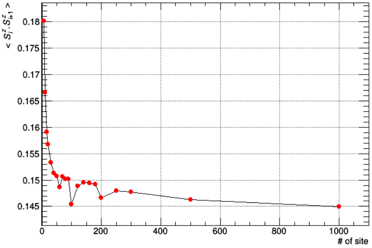
Hubbard Model:

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

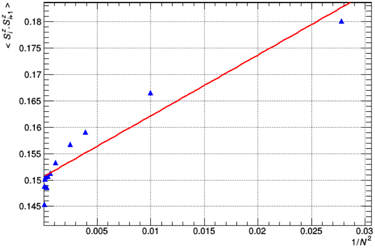
The exactly half filled band case is characterized by a ground state with one electron per site i.e there are no empty sites or holes.The effective Hamiltonian becomes a pure antiferromagnetic Heisenberg Hamiltonian[1]:
$\mathcal{H} = J(t, U) \sum_{<ij>} \mathbf{S_i}.\mathbf{S_j}$

1. Start with an initial state or configuration α of spins.Calculate the spin correlation $S_i^z.S_{i+j}^z$.
2. Vary the configuration by exchanging positions of two electrons with opposite spins randomly to get new configuration $\alpha^{'}$.Calculate the ratio of amplitudes.(vandermonde det)
3. Metropolis aceeptance :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. Compute average:$< S_i^z.S_{i+j}^z >$.

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



(a) Nearest Neighbour spin correlation.



(b) spin correlation vs $1/N^2$

Figure: 1.All 10^6steps

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

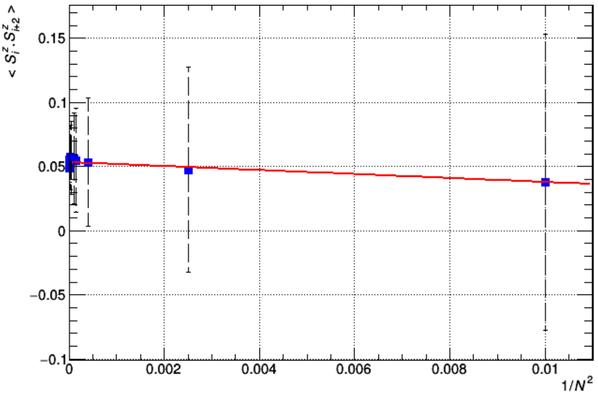


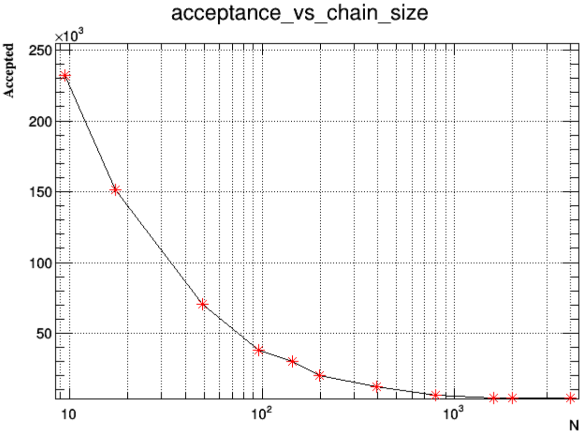
Figure: 2:NN spin Correlation

The error bars are very large compared to nearest neighbour spin correlation. The extrapolated infinite limit NN spin correlation is:
$q_2(\infty) = 0.0533536 \pm 0.008248$.

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.

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

Computational cost:spin-corr::O(N),vandermonde-matrix::O(N)
Accepted=A,Rejected=R then O(A.N^2+RN),where A+R=MC(total monte carlo steps)



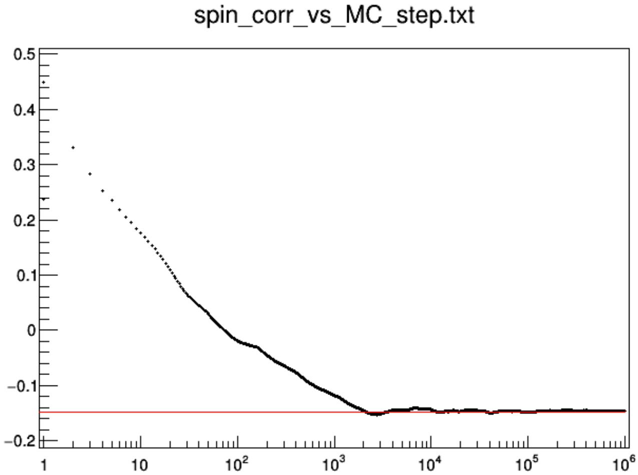


Figure: Chain size=80.MC=10^6