2.1 Noise considerations

We want to consider the statistical fluctuations in the quantity $S_{\boldsymbol{Q}}$ due to the possibly random orientation of the spins. $S_{\boldsymbol{Q}}$ is defined as

$$S_{\boldsymbol{Q}} = \frac{4}{N} \sum_{mn} e^{i\boldsymbol{Q}(\boldsymbol{R}_m - \boldsymbol{R}_n)} S_{zm} S_{zn} \tag{73}$$

Notice that this quantity can also be written as

$$S_{\boldsymbol{Q}} = \frac{4}{N} \sum_{m} e^{i\boldsymbol{Q}\cdot\boldsymbol{R}_m} S_{zm} \sum_{n} e^{-i\boldsymbol{Q}\cdot\boldsymbol{R}_n} S_{zn} = \frac{4}{N} \left| \sum_{m} e^{i\boldsymbol{Q}\cdot\boldsymbol{R}_m} S_{zm} \right|^2 \tag{74}$$

In other words, $S_{\boldsymbol{Q}}$ can be written as the norm squared of a sum over the spin arrangement. When looking at the Bragg angle (that is when $\boldsymbol{Q} = (\pi, \pi, \pi)$) the exponential term in the sum can only take the values ± 1, so the sum will be a real number. If the sample is not ordered, the distribution of the spins in the lattice is completely random and the sum can be represented as the total distance traveled in a random walk where the length of each step is $1/2$ and the probability of taking a step $+1/2$ is $p = 0.5$. When the sample has some order, the random walk will be biased, with $p > 0.5$ in general and $p = 1$ for a completly ordered sample.

To simplify matters let us take the factor of $1/2$ out of the spin variable and consider the random walk with unit step. We have then that

$$\sum_{m} e^{i\boldsymbol{\pi}\cdot\boldsymbol{R}_m} S_{zm} = \frac{1}{2} X_N \tag{75}$$

where X_N is a random variable the represents the total distance traveled in a random walk with unit step after N steps. The probability density function for X_N is a binomial distribution

$$P(X_N = k) = \binom{N}{(N+k)/2} p^{(N+k)/2} (1-p)^{(N-k)/2} \tag{76}$$

which in the limit of a large number of steps can be approximated by a gaussian probability distribution. Using $q = 1 - p$ this is

$$P(X_N = k) = \frac{1}{\sqrt{2\pi}\sqrt{4Npq}} \exp\left[-\frac{1}{2} \frac{(k - N(p-q))^2}{4Npq} \right] \tag{77}$$

The probability density function for X_N^2 can be obtained from $P(X_N = k)$ as

$$\begin{aligned} P(X_N^2 = y) &= \frac{1}{2\sqrt{y}} [P(X_N = \sqrt{y}) + P(X_N = -\sqrt{y})] \\ &= \frac{1}{2\sqrt{y}} \frac{1}{\sqrt{2\pi}\sqrt{4Npq}} \left(\exp\left[-\frac{1}{2} \frac{(\sqrt{y} - N(p-q))^2}{4Npq} \right] + \exp\left[-\frac{1}{2} \frac{(-\sqrt{y} - N(p-q))^2}{4Npq} \right] \right) \end{aligned} \tag{78}$$

where it needs to be kept in mind that $y \geq 0$.

We can go one step further and notice that since

$$S_{\boldsymbol{\pi}} = \frac{X_N^2}{N} \tag{79}$$

the probability density function for $S_{\boldsymbol{\pi}}$ is

$$
\begin{aligned}
P(S_{\boldsymbol{\pi}} = s) &= \frac{\sqrt{N}}{2\sqrt{s}} \left[P(X_N = \sqrt{sN}) + P(X_N = -\sqrt{sN}) \right] \\
&= \frac{\sqrt{N/s}}{2\sqrt{2\pi}\sqrt{4Npq}} \left(\exp\left[-\frac{1}{2} \frac{(\sqrt{sN} - N(p-q))^2}{4Npq} \right] + \exp\left[-\frac{1}{2} \frac{(-\sqrt{sN} - N(p-q))^2}{4Npq} \right] \right)
\end{aligned} \tag{80}
$$

The mean and variance of this probability density function can be calculated analytically by doing the integrals in Mathematica, the results are

$$
\begin{aligned}
\mathrm{Mean}(S_{\boldsymbol{\pi}}) &= N(2p-1)^2 + 4pq \\
\mathrm{Var}(S_{\boldsymbol{\pi}}) &= 16pq(N(2p-1)^2 + 2pq)
\end{aligned} \tag{81}
$$

For a completely random spin distrubution we have $p = 1/2$ which gives $\overline{S_{\boldsymbol{\pi}}} = 1$ and $\delta(S_{\boldsymbol{\pi}}) = \sqrt{\mathrm{Var}(S_{\boldsymbol{\pi}})} = \sqrt{2}$, which is independent of N. This variance is quite large, it is in fact larger than the mean value. In our experiment we take a number of shots n_s, where each shot is a measurement of $S_{\boldsymbol{\pi}}$. If we happend to be looking at an unordered sample ($p = 0.5$), the uncertainty in the mean of $S_{\boldsymbol{\pi}}$ is then given by

$$
\delta\left(\overline{S_{\boldsymbol{\pi}}}\right) = \sqrt{2/n_s} \tag{82}
$$

If we want this uncertainty to go to the 0.1 level we would need to average $n_s = 2/(0.1^2) = 200$ shots. We typically take some 10 shots, which for an unordered sample gives us $\delta\left(\overline{S_{\boldsymbol{\pi}}}\right) = 0.44$.

2.1.1 Random realizations of $S_{\boldsymbol{\pi}}$

We have run some numerical tests with sets of randomly ordered spins. The results from evaluating $S_{\boldsymbol{\pi}}$ numerically can be compared with the probability density function obtained in the previous section, this comparison in shown in Fig. 1.

2.1.2 Results for an AFM ordered core

We can also consider a sample which has an AFM ordered domain of size L_{AFM} at the center and then a randomly ordered shell on the outside. Care is taken to make sure the spin mixture is balanced. Numerically realizing random distributions of the spins in the shell we can obtain the distributions of $S_{\boldsymbol{\pi}}$ as a function of system size and size of the AFM domain. The results are shown in Fig. 2.

The mean values of the expected results at our detection cameras are shown for various values of N and L_{AFM} in Fig. 3.

By plotting the mean, standard deviation and their ratio for the quantity $S_{\boldsymbol{\pi}}$ we can see that the relative fluctutations only go down for values of $S_{\boldsymbol{\pi}}$ significantly larger than 1, which is a regime that would only be attained below the Neel transition. This is shown in Fig. 4.

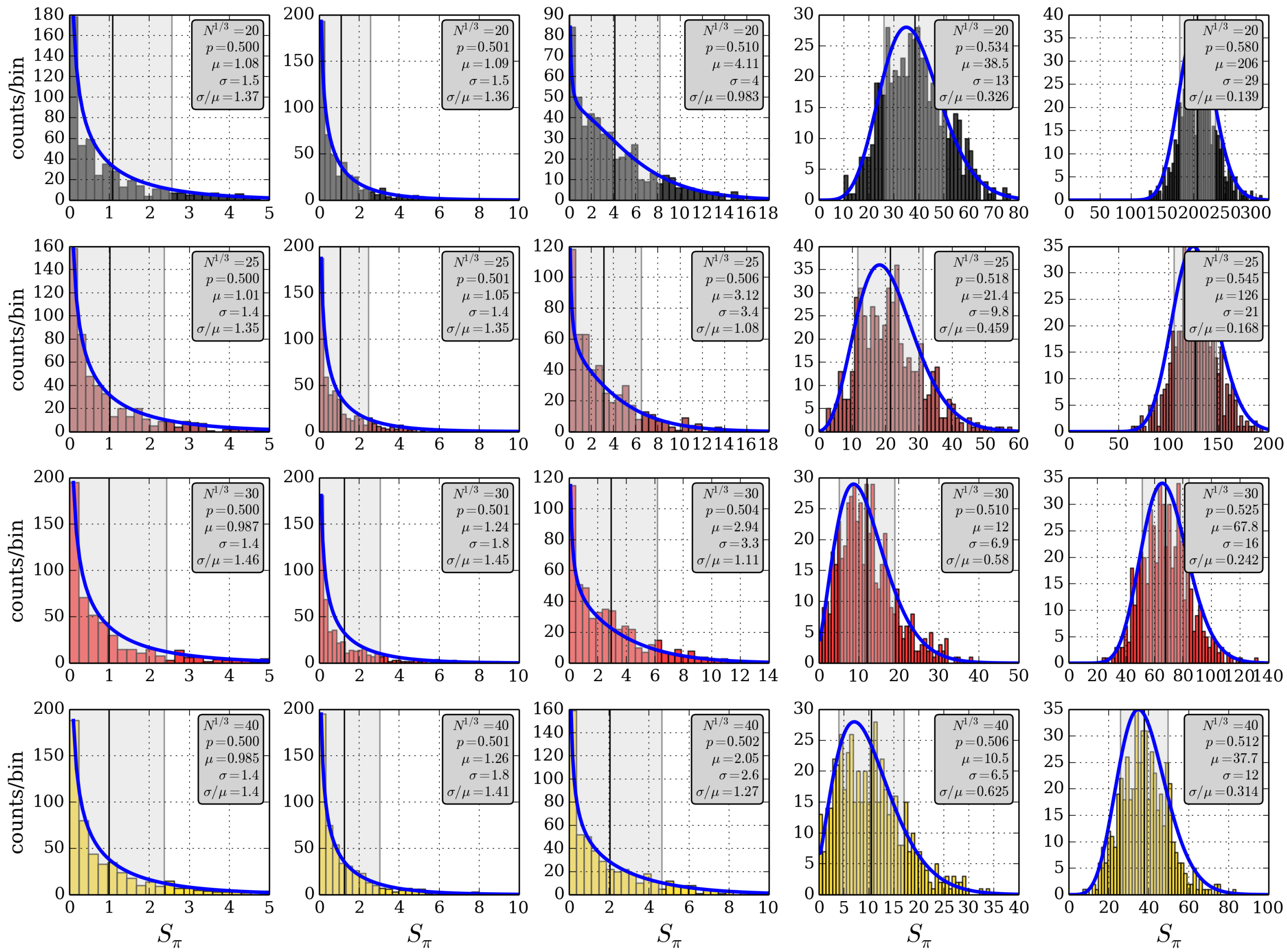

Figure 1: Distribution of $S_{\boldsymbol{\pi}}$ for randomly ordered spins. The spin ordering is parameterized by the parameter p as described in the text. The probability density function $P(S_{\boldsymbol{\pi}})$ as derived in the text is shown by the blue line. The thin black line denotes the mean of the distribution and the shaded gray area denotes ± 1 standard deviations.

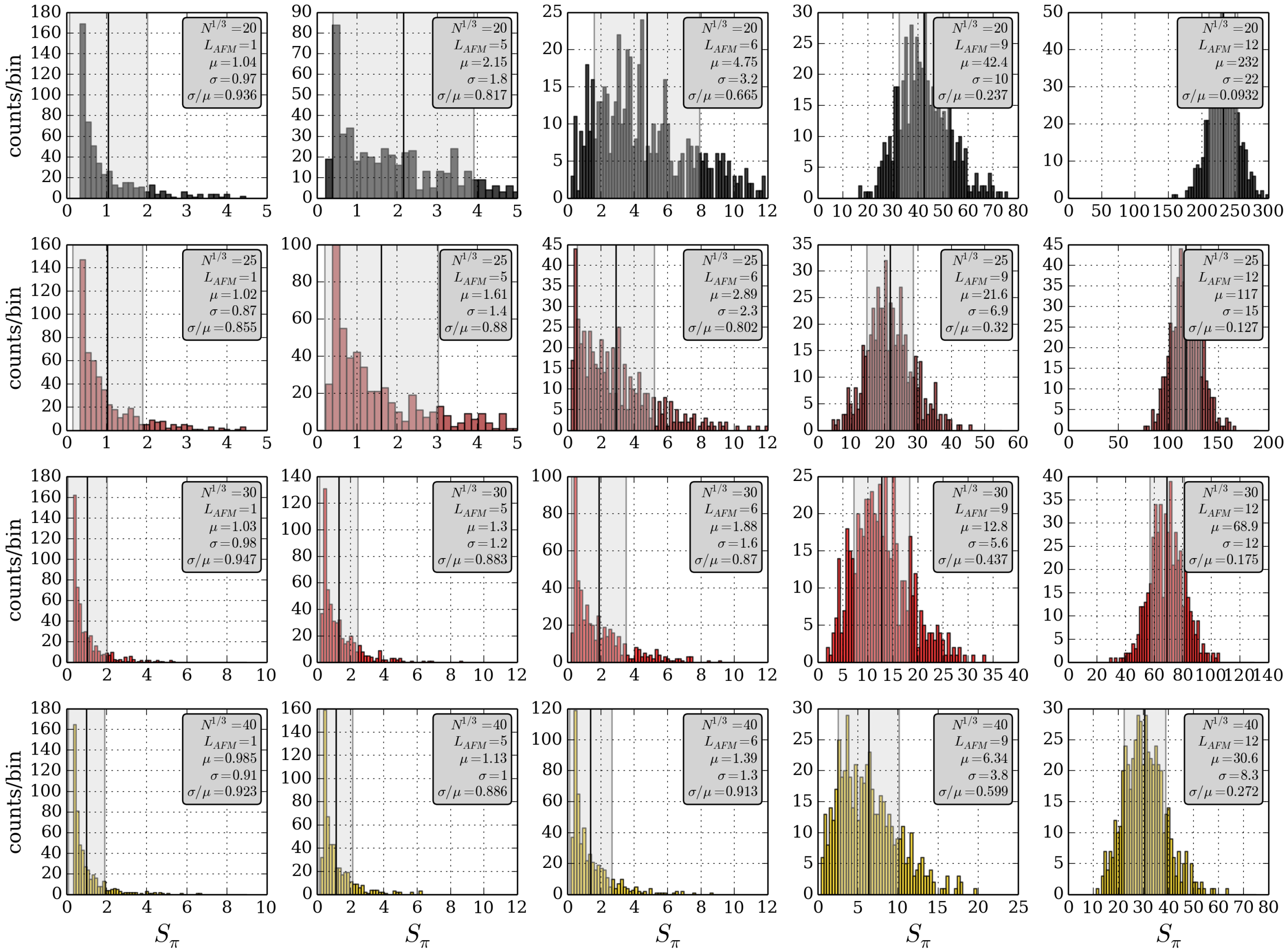

Figure 2: Distribution of $S_{\boldsymbol{\pi}}$ for randomly ordered spins. The spin ordering is parameterized by the size of the AFM domain as described in the text. The thin black line denotes the mean and the shaded gray area denotes ± 1 standard deviations.

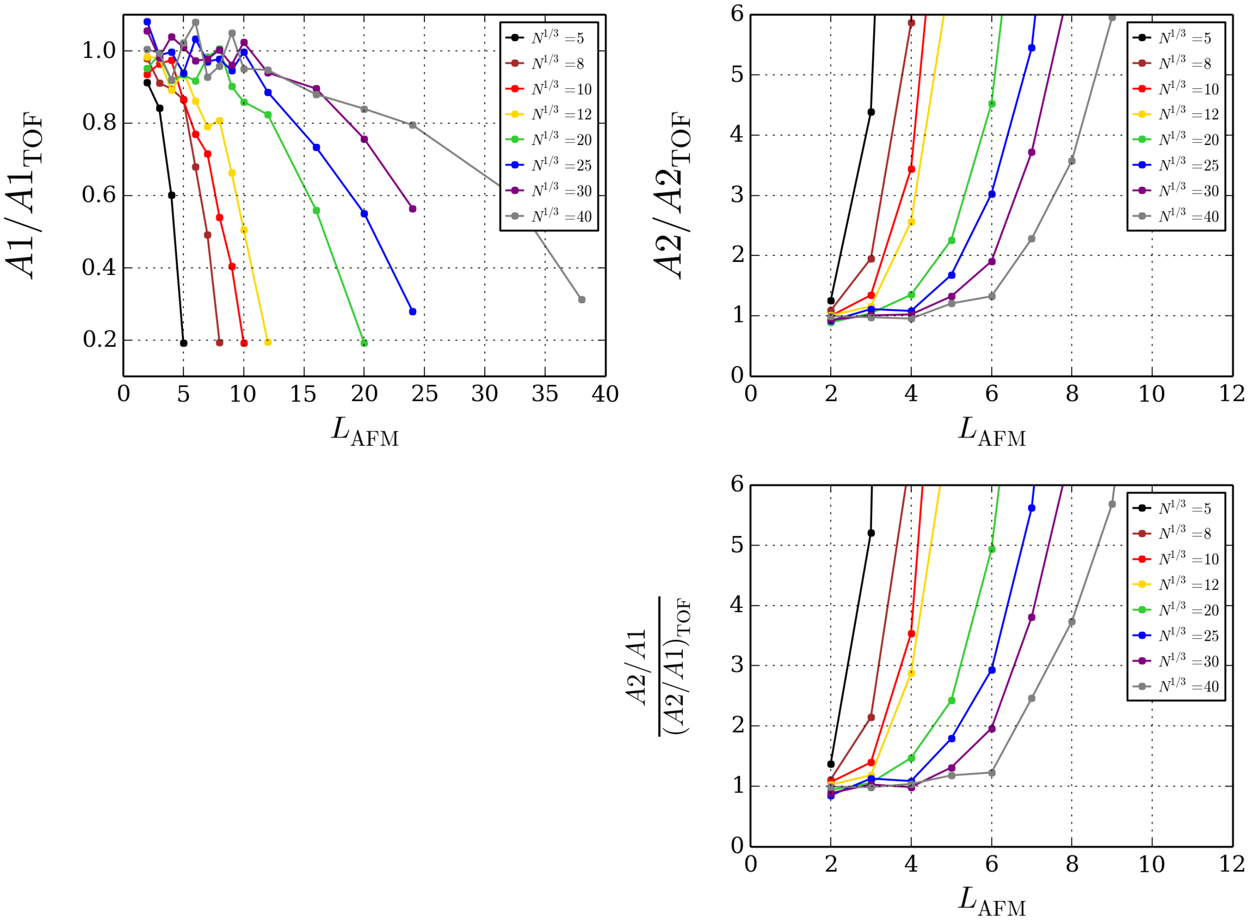

Figure 3: Mean value of $S_{\boldsymbol{\pi}}$ for randomly ordered spins. The spin ordering is parameterized by the size of the AFM domain as described in the text.

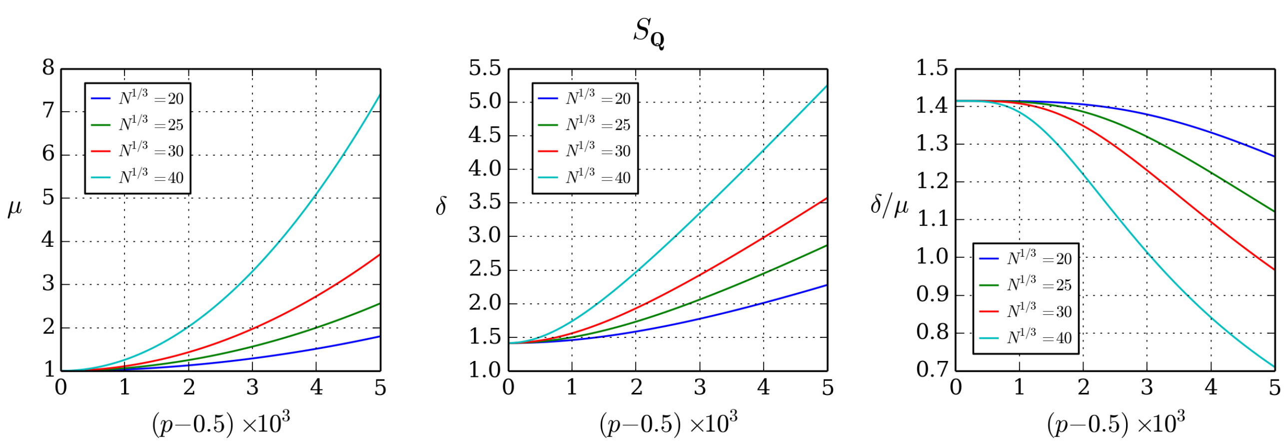

Figure 4: Mean value, variance, and their ratio for $S_{\boldsymbol{\pi}}$ are plotted for different values of p, and N.