Step Analysis

We have already established the independence of individual steps in a parallel environment as

$$p(a \to b) = p(a \to c) \cdot p(c \to b)$$

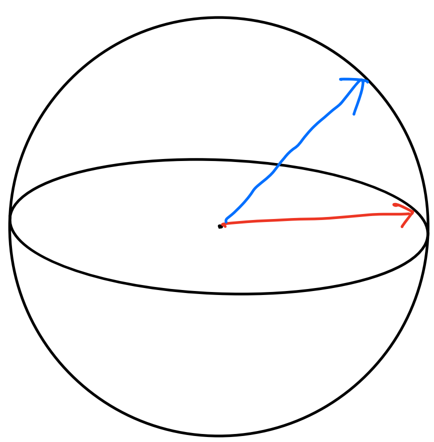
The energy shift (dE) per MCS would follow certain trends.

Since our Hamiltonian is large, let us consider a simplified Hamiltonian as

$$H = -\frac{1}{2} J \sum \vec{S}_i \cdot \vec{S}_j$$

Taking only the point of interest i

we get
$$H_i = -J \sum \vec{S}_i \cdot \vec{S}_{i_{adj}}$$
$$H_i = -J \, \underline{\vec{S}_i} \cdot \underline{\sum \vec{S}_{i_{adj}}}$$



$$dE = -J \, d\vec{S}_i \cdot \vec{S}_{i_{adj}}$$

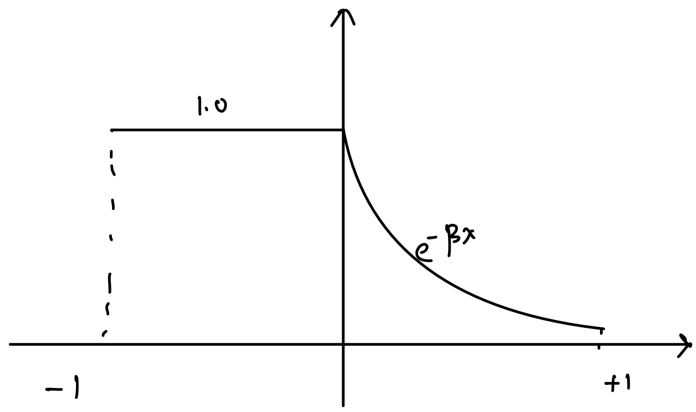
now, this can take a value between $J[-1, 1]$, considering unit vectors.

For simplification, take $J = 1 \Rightarrow dE \in [-1, 1]$

Now, from the metropolis criteria,

if $dE \leq 0 \rightarrow p(dE) = 1.0$

$dE > 0 \rightarrow p(dE) = e^{-\beta dE}$



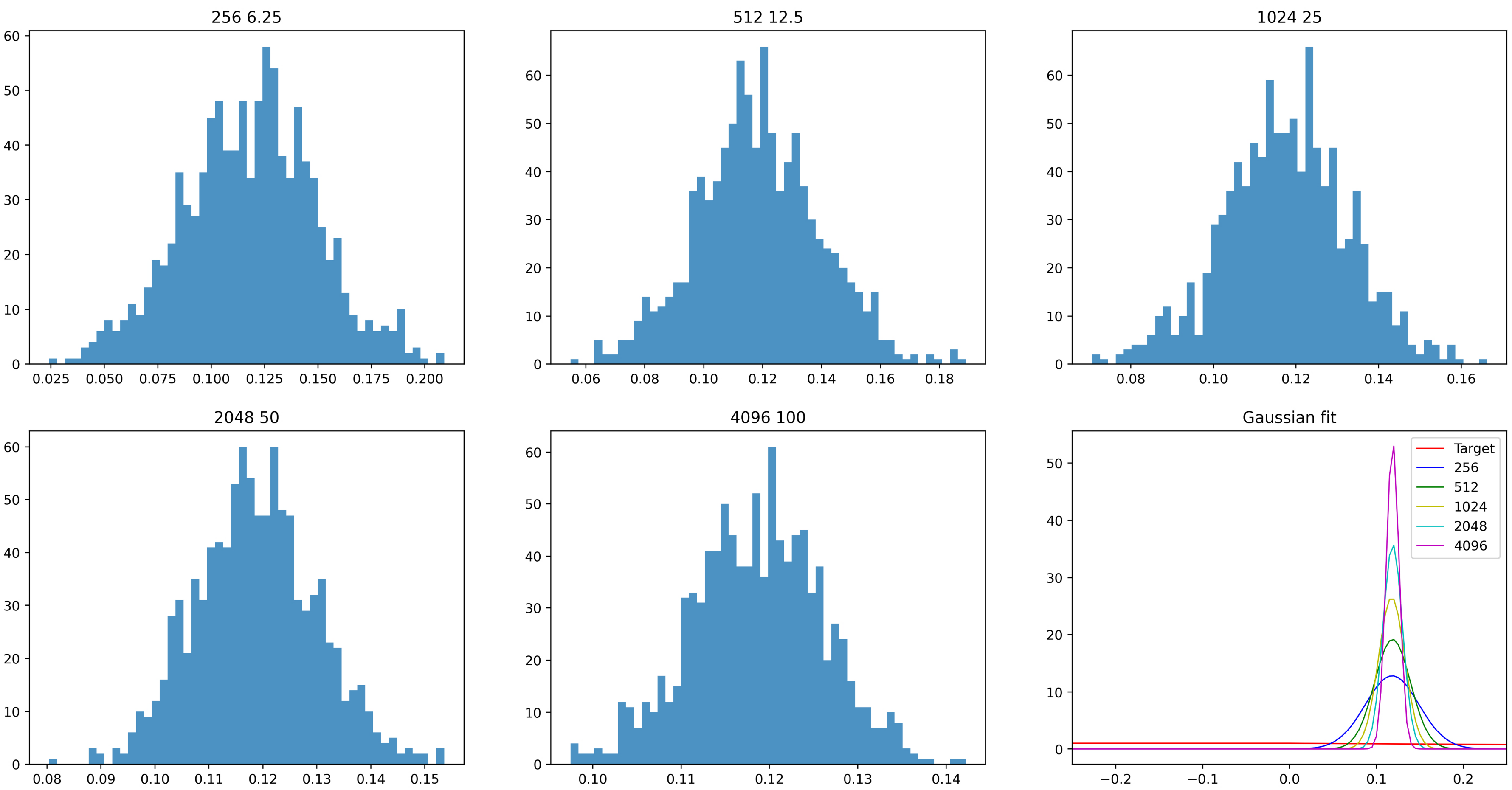
This is the sample space of dE, or our energy shift / metropolis.

For our purposes, $\Delta E_{mcs} = \prod^{P} p_i(dE)$ from the above distribution.

The results are given below as a function of P with a linear target depicting uniform distribution.

Observations

We see a greater shift in the fit gaussian in low P with spikes in higher P signaling lower dE steps


256 6.25
512 12.5
1024 25
2048 50
4096 100
Gaussian fit
Target
256
512
1024
2048
4096