1 The Hamiltonian

We are looking at a bilayer Heisenberg spin model where each layer contains $N \times N$ spins. The Hamiltonian is

$$H = H_{intra} + H_{inter} + H_{an} + H_{ext} \tag{1}$$

where the *intralayer exchange interaction* term is

$$H_{intra} = -\sum_{l}\sum_{<i,j>} J_{intra,ij}\vec{S}_i^{(l)} \cdot \vec{S}_j^{(l)}$$

where the sum is taken over nearest neighbors within the same layer, indicated by l. The minus sign out front indicates that a strong, positive $J_{intra,ij}$ causes intralayer alignment to be energetically favorable. The intralayer exchange interaction strength $J_{intra,ij}$ is the same for all pairs i, j so we can simply write

$$H_{intra} = -J_{intra}\sum_{l}\sum_{<i,j>} \vec{S}_i^{(l)} \cdot \vec{S}_j^{(l)}$$

The *interlayer exchange interaction* term is

$$H_{inter} = J_{inter}\sum_{i} \vec{S}_i^{(1)} \cdot \vec{S}_i^{(2)}$$

The sum is taken over all lattice sites and the interaction takes place between corresponding spins on the same site in each layer. The *anisotropic* term is

$$H_{an} = k\sum_{l}\sum_{i}\left(S_{i,z}^{(l)}\right)^2$$

where a negative k value indicates easy axis anisotropy along the z axis. The external field term is

$$H_{ext} = -B\sum_{l}\sum_{i} S_{i,z}^{(l)}$$

The full Hamiltonian is therefore

$$\boxed{H = -J_{intra}\sum_{l,<i,j>} \vec{S}_i^{(l)} \cdot \vec{S}_j^{(l)} + J_{inter}\sum_{i} \vec{S}_i^{(1)} \cdot \vec{S}_i^{(2)} + k\sum_{l,i}\left(S_{i,z}^{(l)}\right)^2 - B\sum_{l,i} S_{i,z}^{(l)}}$$

2 The Free Energy

The free energy is calculated using

$$F = U - TS$$

In the mean field approximation, we take the average of the Hamiltonian. We first make the observation that there is no inter-layer planar interaction, so within a given layer, we expect all spins within a layer to be aligned in the same direction (at low T). Therefore, the exchange interaction term is constant.

$$H = -J_{intra}(4N^2) + J_{inter} \sum_i \vec{S}_i^{(1)} \cdot \vec{S}_i^{(2)} + k \sum_{l,i} \left(S_{i,z}^{(l)} \right)^2 - B \sum_{l,i} S_{i,z}^{(l)}$$

where each layer is of $N \times N$ size. Secondly, we observe that since every spin within a layer behaves in the same way, we can reduce the analysis to that of a single spin in each layer. So, we will analyze the behavior of the following simplified Hamiltonian

$$\begin{aligned} H &= J_{inter}(\vec{S}^{(1)} \cdot \vec{S}^{(2)}) + k \sum_l \left(S_z^{(l)} \right)^2 - B \sum_l S_z^{(l)} \\ &= J_{inter}(\vec{S}^{(1)} \cdot \vec{S}^{(2)}) + k((S_z^{(1)})^2 + (S_z^{(2)})^2) - B(S_z^{(1)} + S_z^{(2)}) \end{aligned}$$