EFM With Field in 110 Starting With Random and Ground Initial States

May 5th, 2016 - May 25th, 2016

Andrew Way

Overview

The effective field method was used to 2000 iterations to determine the 0 temperature states of the 12x12x12 3D FCC kagome lattice while being subjected to a changing magnetic field along the 110 direction. The field was either incremented or decremented in steps of 0.0001. There were 4 cases studied:

1. **Increasing** magnetic field in the **110** direction from **0.00 to 0.05**, with an initial spin configuration that was a **ground state** with theta = 0.206275 and phi = 3.11867.
2. **Increasing** magnetic field in the **110** direction from **0.00 to 0.05**, with an initial spin configuration that was **randomly generated**.
3. **Decreasing** magnetic field in the **110** direction from **0.05 to 0.00**, with an initial spin configuration that was a **ground state** with theta = 0.206275 and phi = 3.11867.
4. **Decreasing** magnetic field in the **110** direction from **0.05 to 0.00**, with an initial spin configuration that was **randomly generated**.

Analysis that was performed on the resulting data included the following:

- Plots of magnetization versus field
- Plots of energy versus field
- Animations of the characteristic 6 spins
- Determination of the number of "unique" spins that populate the lattice
- Determination of the components of the unique spins
- Plots of azimuth and zenith angles of the A, B, C, D, E, and F spins w.r.t. the plane of the 111 normal vector

RUN 1: Increasing Field, Ground State

Two inflection points are evident in the graphs of energy and magnetization, indicating the occurence of a sudden change in orientation of the spins. The first inflection point occurs at H 0.005, at which the spins snap into a planar state. The second occurs at H 0.009, where another planar state forms but oriented in a different direction. From thereon out, the spins gradually align with the 110 field and nothing else interesting happens.

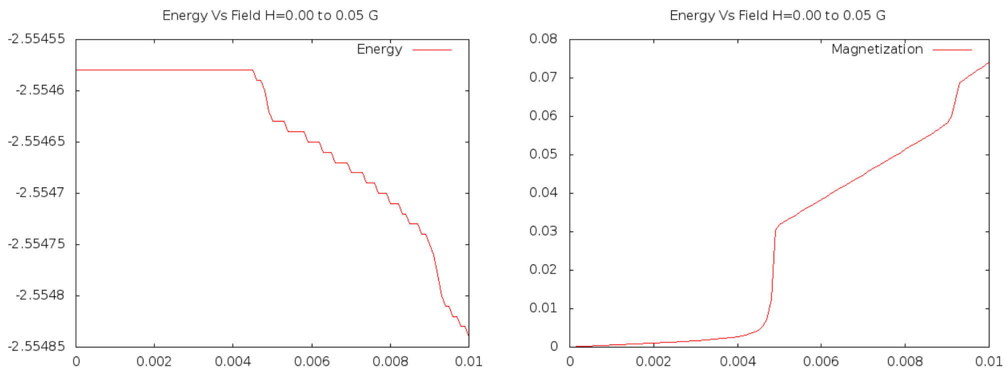


Figure 1: Energy vs increasing field and Magnetization versus increasing field

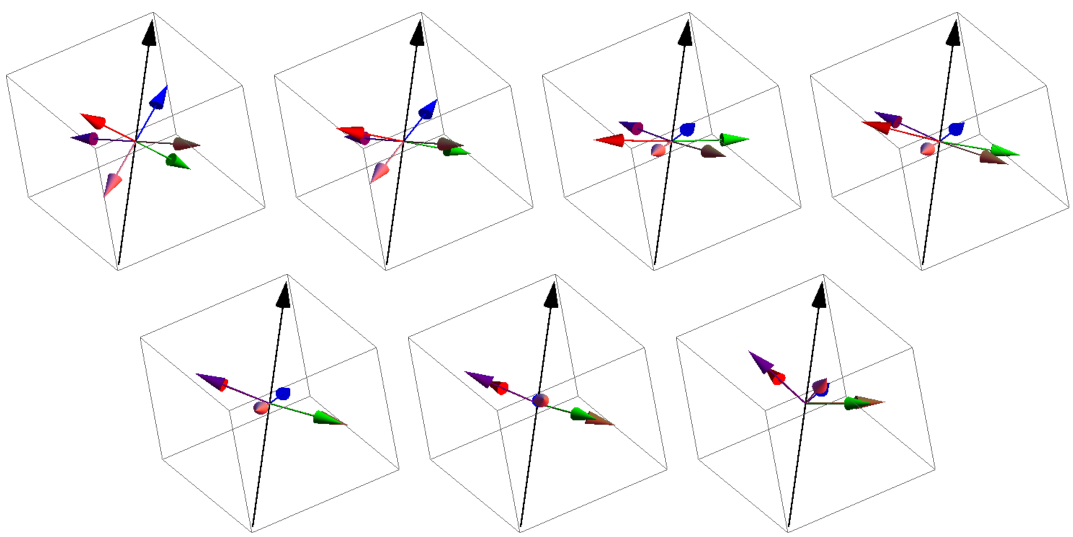
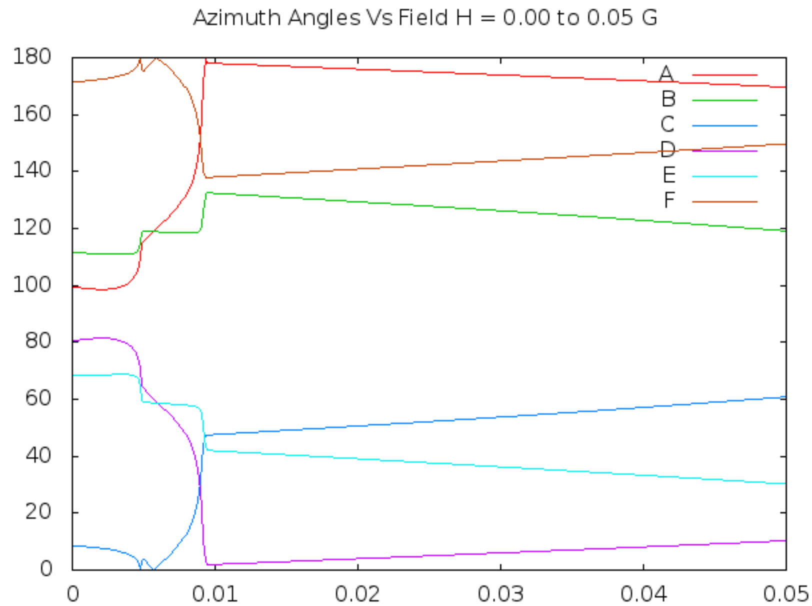


Figure 2: Snapshots of the 6 characteristic spins of the lattice at H=0, 0.0046, 0.0052, 0.0082, 0.0091, 0.0097, and 0.05



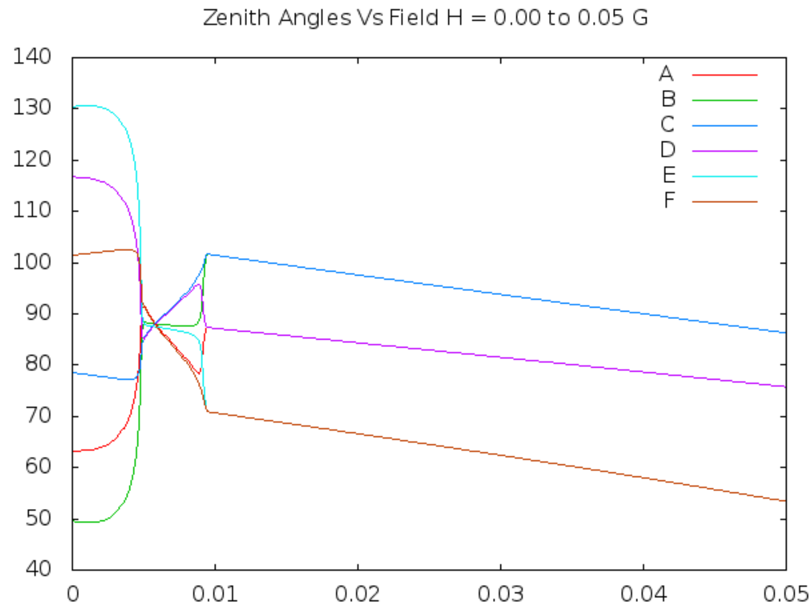


Figure 3: The angles are those between a chosen vector lying in the plane intersected by 111, and a projection of each of the A, B, C, D, E, and F spins. Azimuthal angles are followed by zenith angles.

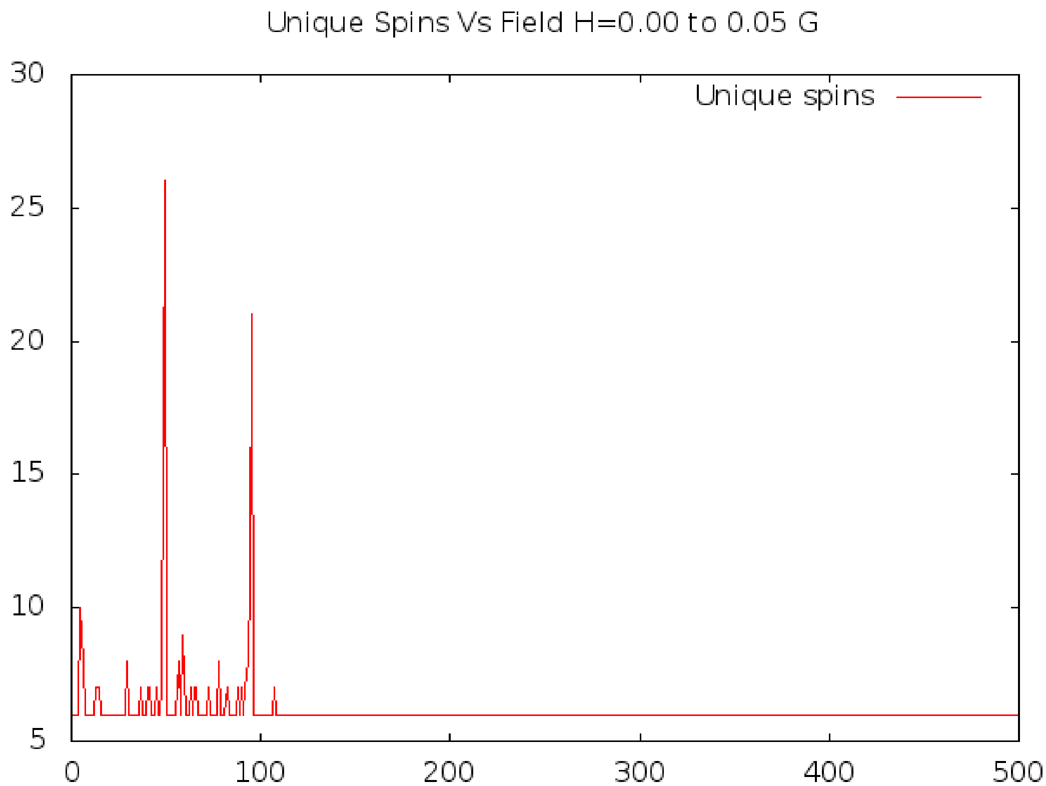


Figure 4: Peaks in the number of unique spins at approx. 0.05 and 0.09, indicating the occurence of transitions.

RUN 2: Decreasing Field, Ground State

Similar to starting with a high field in the 111 direction, the spins are in a planar state that is aligned with the field. When the field is lowered, the spins are stuck in a planar state. In the first snapshot of the spins, the brown and green spins are partially aligned. This is likely due to insufficient number of iterations for EFM. 3000 steps is typically sufficient, while 2000 is not.

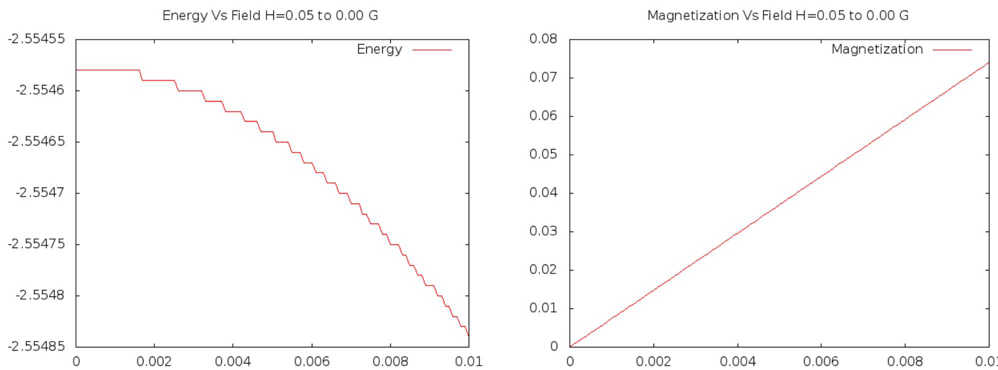


Figure 5: Energy vs decreasing field and Magnetization versus decreasing field

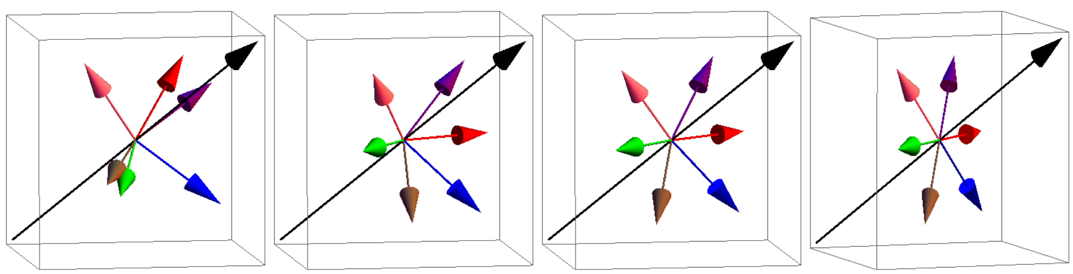


Figure 6: Snapshots of the 6 characteristic spins of the lattice at B=0.05, B=0.0418, B=0.0157, and B=0.00

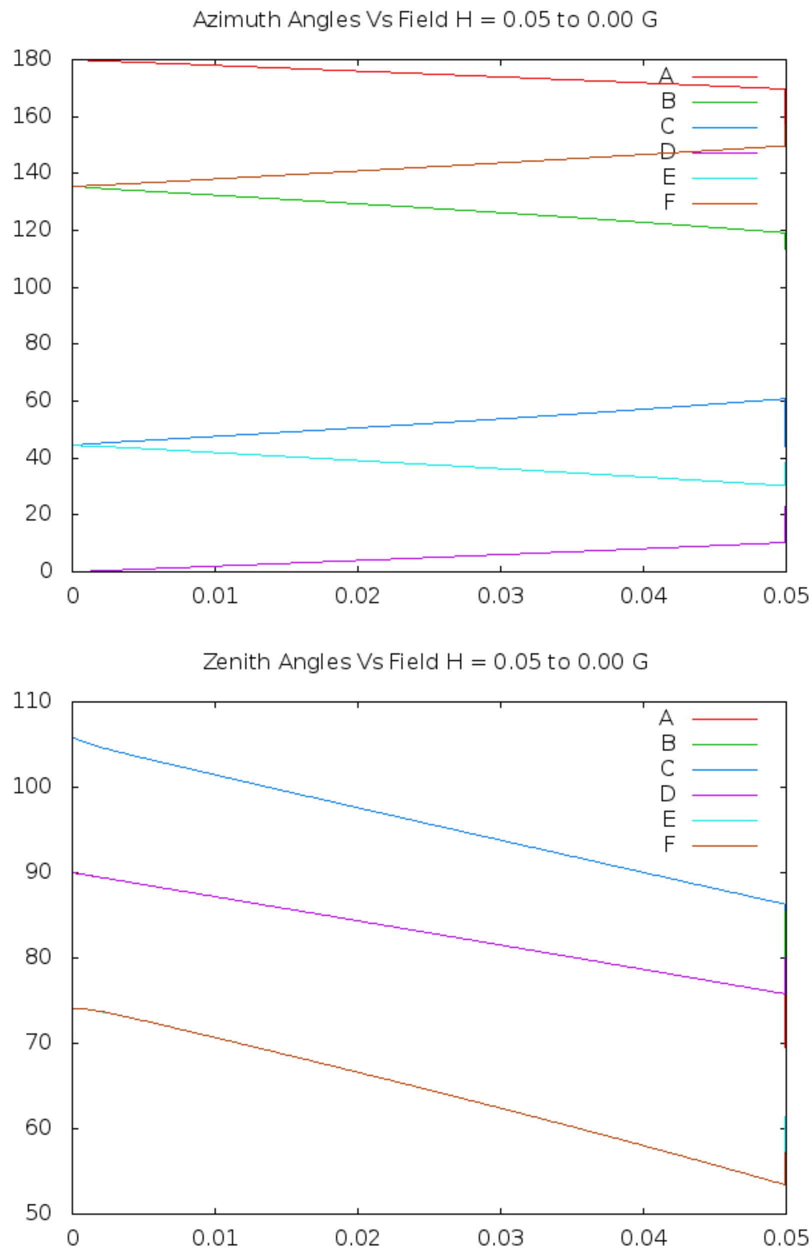


Figure 7: The angles are those between a chosen vector lying in the plane intersected by 111, and a projection of each of the A, B, C, D, E, and F spins. Azimuthal angles are followed by zenith angles.

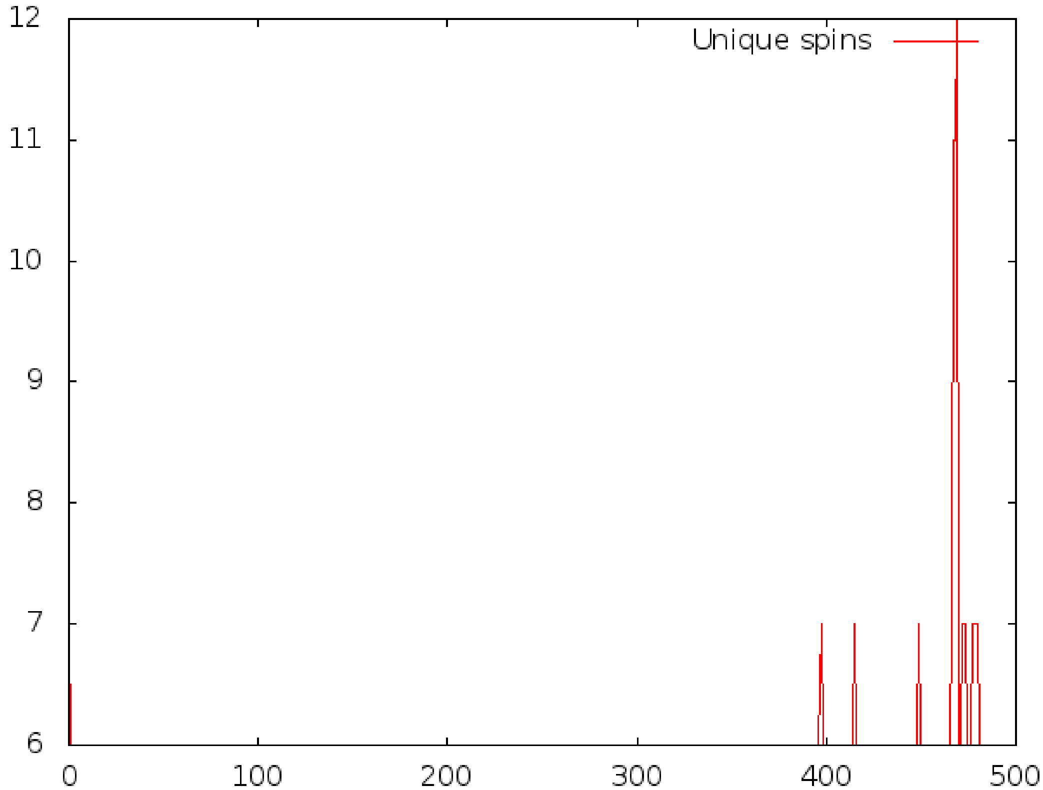
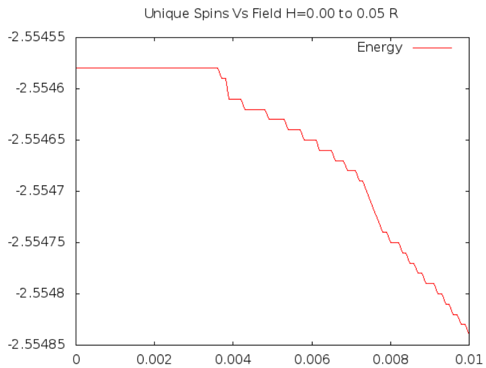


Figure 8: A peak in the number of unique spins at approx H = 0.007, yet no transition occurs in the lattice.

RUN 3: Increasing Field, Random State

Very similar to run 1, in that there are 2 transitions at approximately 0.0038 and 0.0075. The transformation of the 6 spins is similar as well, with the spins beginning in the groundstate, transition to a planar state, 2 pairs of spins rotate and switch places, and the plane the spins lie in reorients itself. The spins then gradually align with the field, and nothing else interesting happens.



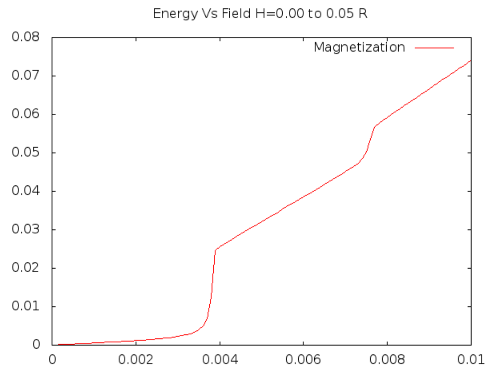


Figure 9: Energy vs increasing field and Magnetization versus increasing field

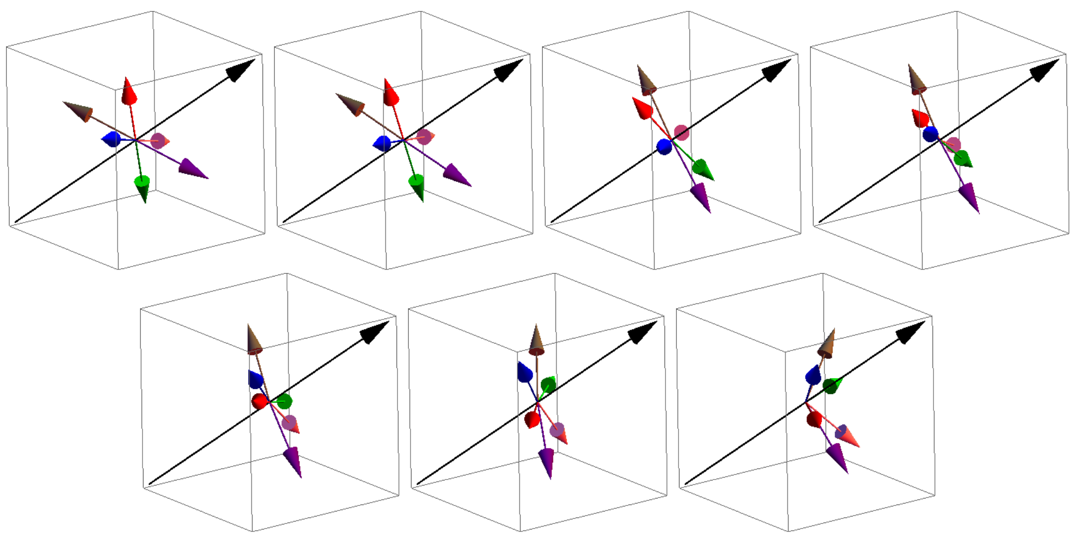


Figure 10: Snapshots of the 6 spins at H = 0.00, 0.0032, 0.0041, 0.0068, 0.0075, 0.0081, and 0.05

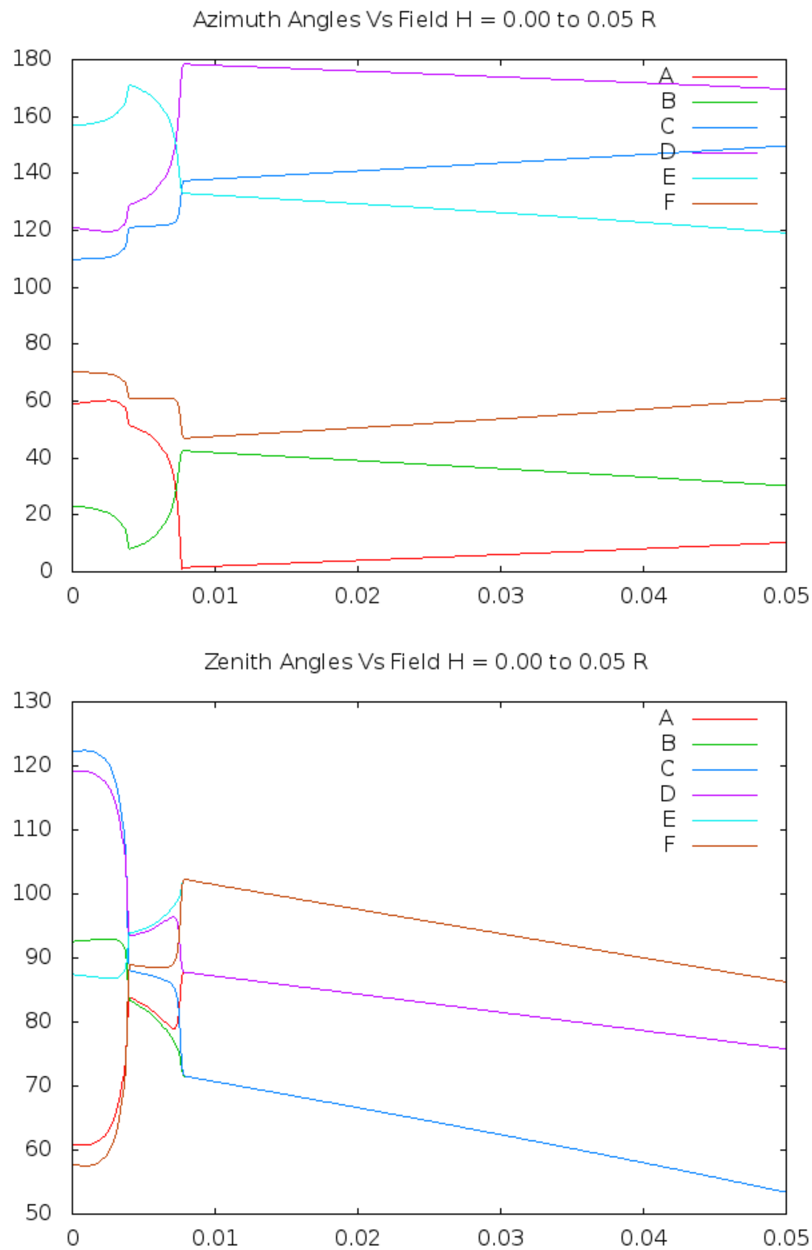


Figure 11: The angles are those between a chosen vector lying in the plane intersected by 111, and a projection of each of the A, B, C, D, E, and F spins. Azimuthal angles are followed by zenith angles.

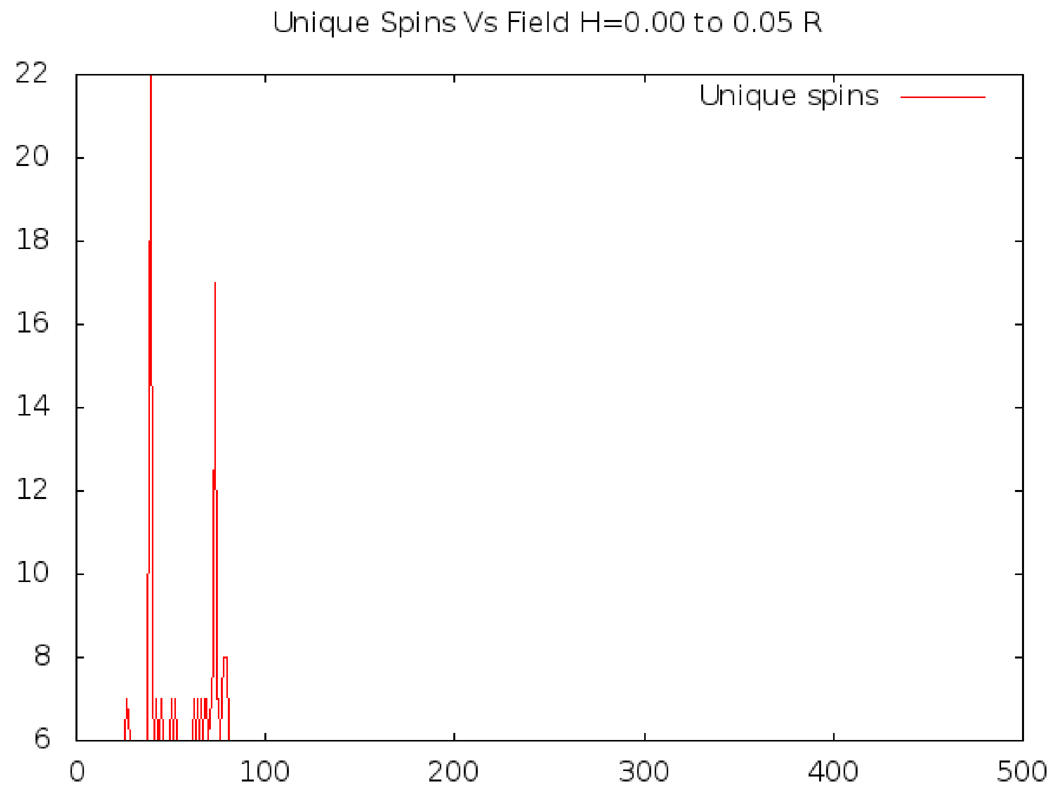


Figure 12: A peak in the number of unique spins occurs at approximately 0.0038 and 0.0075

RUN 4: Decreasing Field, Random State

A sudden transition occurs at approximately 0.022. The green and pink spins swap places with another, and the blue and red spins also follow this swap. It's possible this transition only occurs because there is insufficient steps being used for EFM, as was the case with applying the field in the 111 direction. Any transitions disappeared when increasing the number of steps from 2000 to 3000 steps when decreasing the field with a random initial configuration.

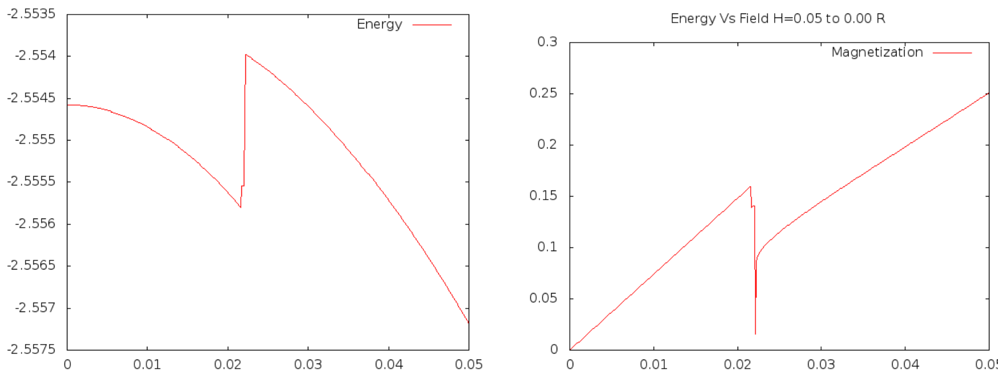


Figure 13: Energy vs decreasing field and Magnetization versus decreasing field

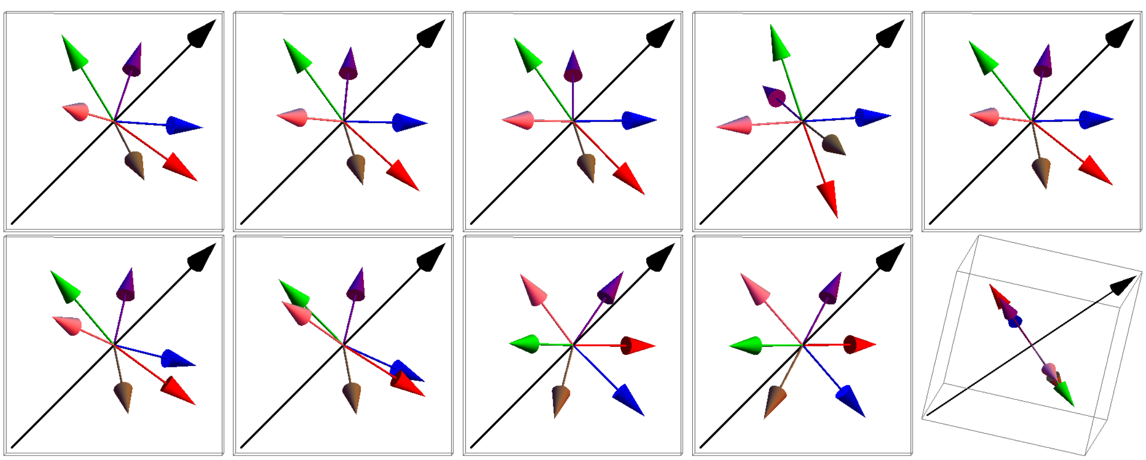


Figure 14: Snapshots of the 6 characteristic spins at H = 0.05, 0.0257, 0.0224, 0.0221, 0.0220, 0.0218, 0.0217, 0.0216 and 0.00. An alternate view of the spins at H = 0.00 is also shown.

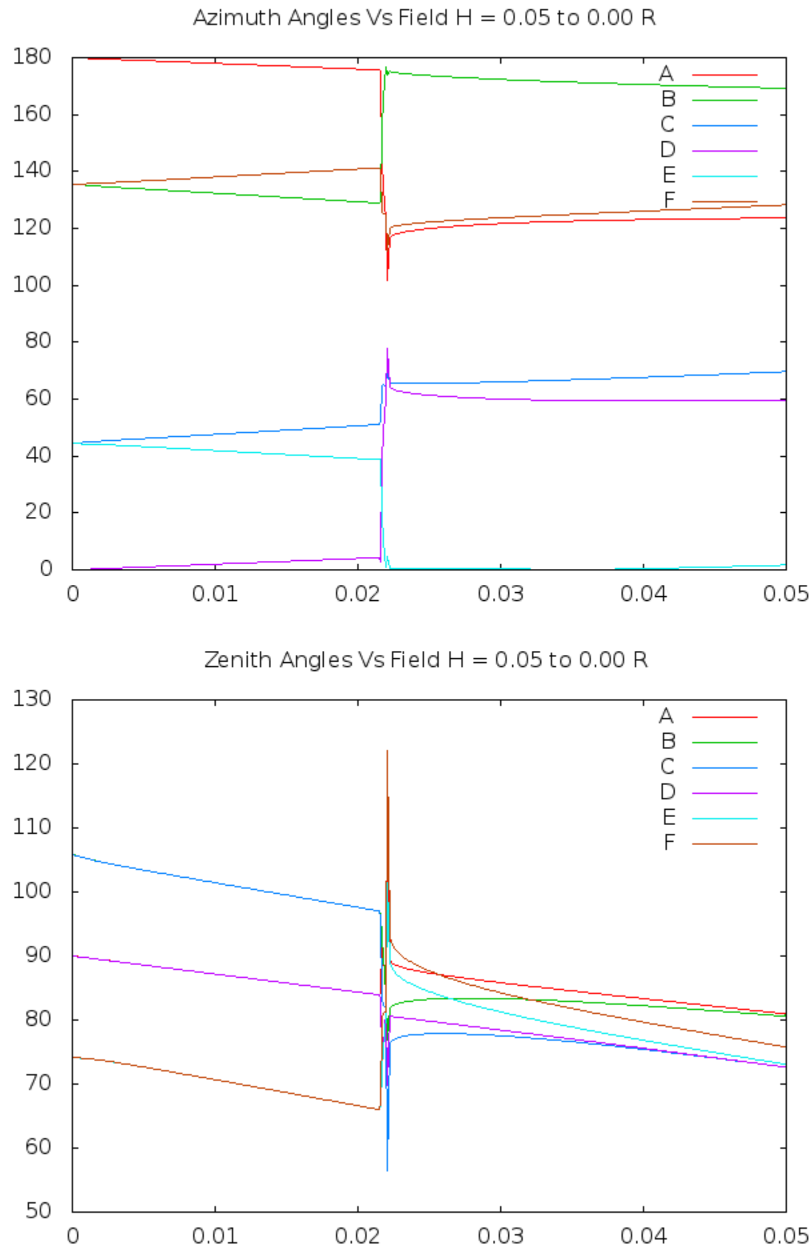


Figure 15: The angles are those between a chosen vector lying in the plane intersected by 111, and a projection of each of the A, B, C, D, E, and F spins. Azimuthal angles are followed by zenith angles.

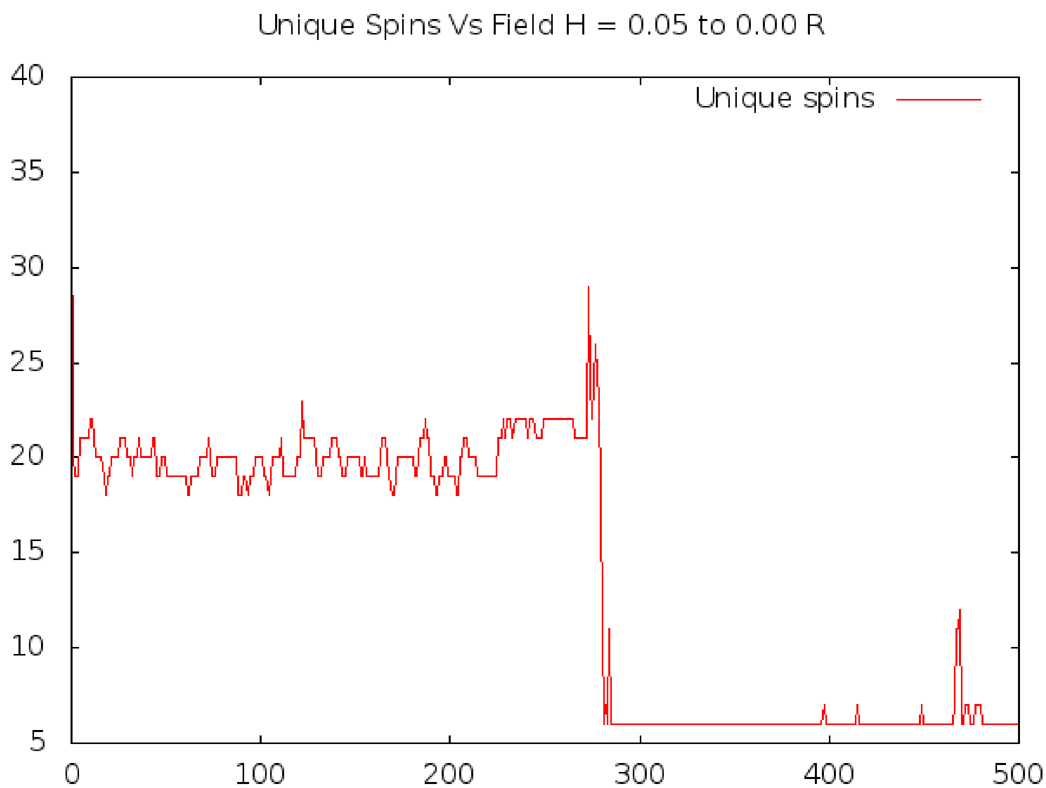


Figure 16: The lattice is highly disordered from H = 0 to H = 0.029. A six spin system is finally achieved after this point.

Appendices

Appendix A - Finding Unique Spins

Overview The azimuth angles are found by projecting each of the 6 chosen spins into the 111 plan and dotting the projections with the (1,-1,0) vector; a vector that lies in the 111 plane. The zenith angles are found by dotting each of the spins with the 111 normal vector.