

# Effective Field Method at Zero Temperature with Field Along Various Directions

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# 1 Introduction

The effective field method was used to 3000 iterations (except where noted) to determine the 0 temperature states of the 12x12x12 3D FCC kagome lattice while being subjected to a changing magnetic field along various field directions.

There are several types of runs which differ in either the starting state, the field direction, the maximum field to which the field was increased, and whether the field was then decreased after being saturated. When starting from a ground state for any of the simulations included in this pdf, the ground state had characteristic angles theta = 0.206275 and phi = 3.11867.

The purpose of these simulations was to observe the behaviour of the lattice's properties when subject to fields of various conditions. Analyses that was performed on the resulting data included the following:

- Plots of magnetization versus field
- Plots of energy versus field
- Composite plots of energy for both increasing and decreasing fields
- Composite plots of magnetization for both increasing and decreasing fields
- Snap shots of the characteristic 6 spins for each lattice at significant points of each simulation
- Determination of the number of “unique” spins that populate the lattice
- Determination of the components of the unique spins
- Dot products of each of the 6 spins with their respective “*neighbors*”.

Preliminary results providing insight on the causes of particular spin configurations due to application of field are also contained within the PDF.

**Note:** In all 6-spin snapshots, the spins are as such: A-Red, B-Green, C-Blue, D-Pink, E-Brown, F-Purple. Determining the number of unique spins that populate a particular lattice was not done for all simulations, but so far it seems that the lattice always maintains a 6 spin system, except during unstable periods in which the lattice undergoes a transition. It's likely that if the number of iterations used for EFM were increased and reran for transition phases the number of unique spins would probably reduce to 6. In other words, I think the system is changing too quickly for EFM with 3000 iterations to properly find its ground state during transitions.

## 2 (001) Increasing Field, Ground State

The 6 spins begin to transition to the planar state at  $H=0.0105$  and achieves the planar state at  $H=0.0121$ . The pink and brown spins swap positions, as do the blue and purple spins, as the field is increased beyond the planar state. The spins gradually align with the 001 field direction, until approximately at 0.14 the lattice becomes saturated and the red and green and spins become parallel to the field direction.

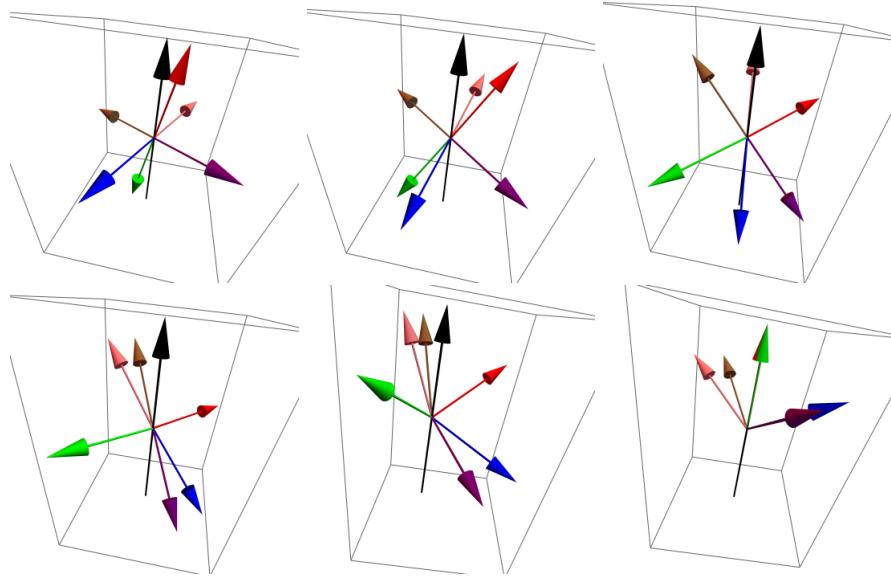
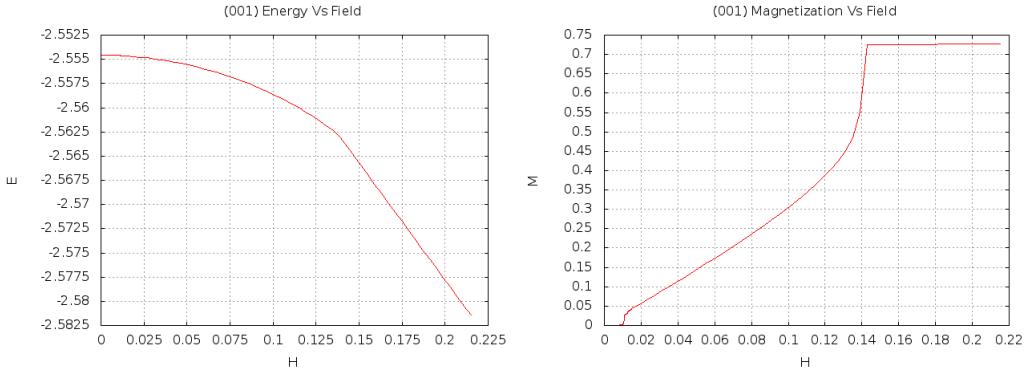


Figure 1: Snap shots of the 6 characteristic spins at  $H=0, 0.0105, 0.0121, 0.0150, 0.131, 0.151$ . The black arrow indicates the direction of the field. In the dot product graph,  $AB$  dot product goes to zero once the lattice is saturated. This agrees with  $A$  and  $B$  (red and green) lining up in the above snapshots.

### 3 (001) Decreasing Field, Ground State

The lattice leaves the saturated state at a field lower than what was required to induce it while increasing the field. This transition from saturation occurs at approximately  $H=0.13$ , compared to the transition to saturation at  $H=0.14$  when increasing the field. The spins gradually unalign and rest in a planar state at zero field, and is characterized by the groundstate angles  $\theta=89.9$  degrees and  $\phi=44.94$  degrees.

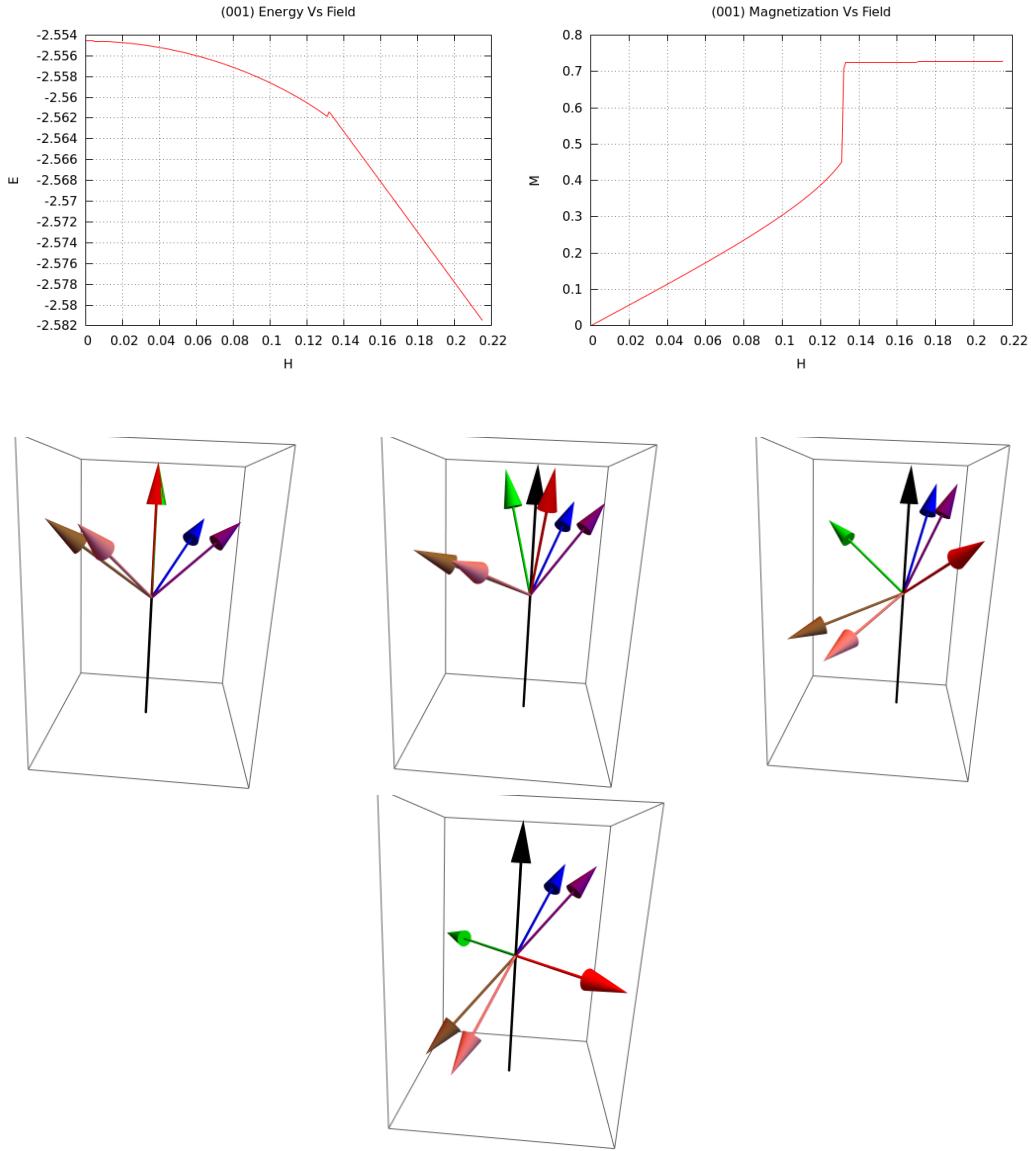


Figure 2: Snapshots at  $H=0.215, 0.132, 0.130, 0$

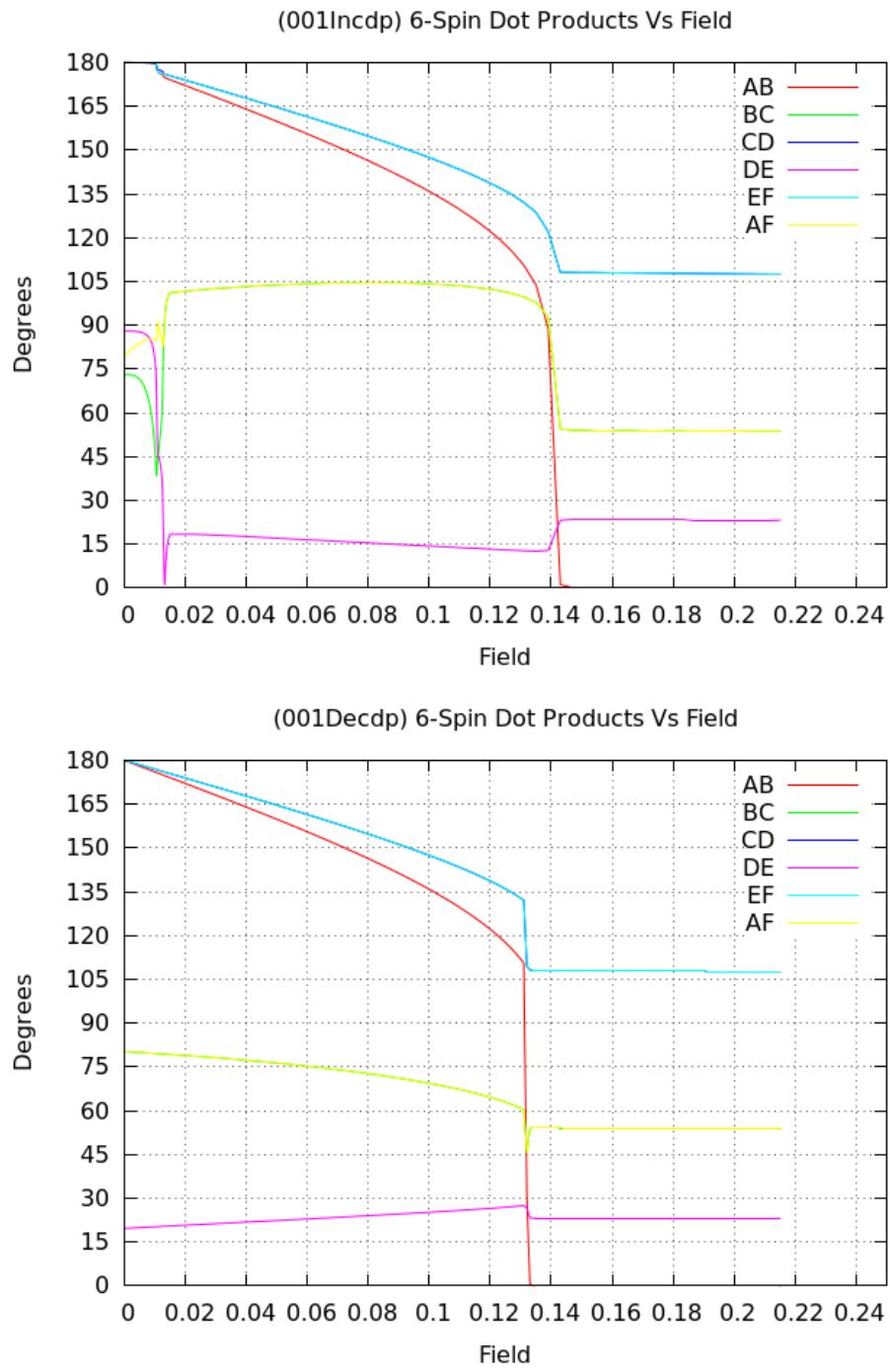


Figure 3: Dot products between the characteristic spins for both increasing and decreasing field.

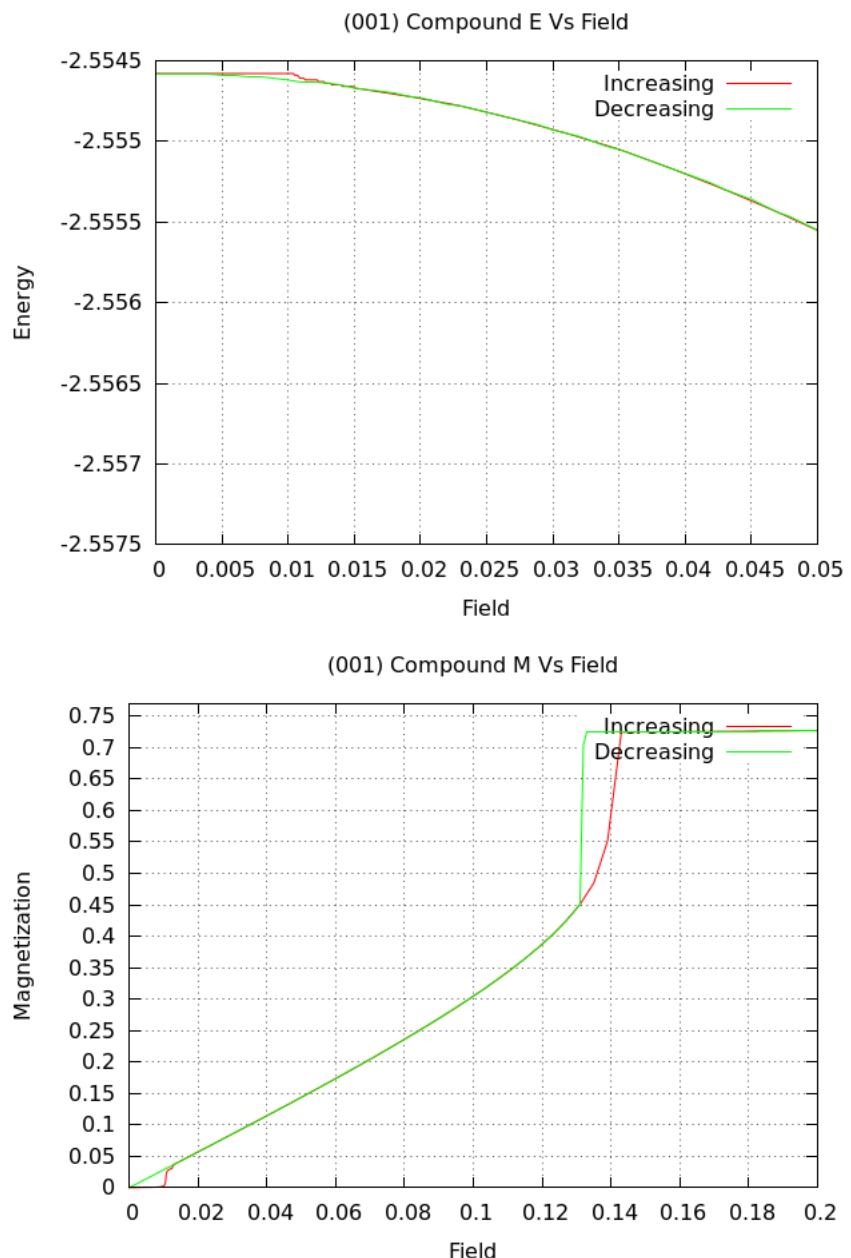


Figure 4: Composite graphs of energy and magnetization for both decreasing and increasing field magnitude. Note the different scales for the energy and magnetization graph. This is because plotting energy vs field on a graph which has an xrange of 0.2 reduces the ability to see any difference in the energy curves. This was done for all composite graphs.

## 4 (010) Increasing Field, Ground State

The lattice begins to undergo a transition at 0.0110. At 0.0114 the planar state is achieved. Similar to 001, two pairs of spins begin to swap positions at around 0.015, though the pairs consist of spins different from 001. The blue and green spins and red and pink spins appear to be swapping positions, but never do. The spins gradually align with the 010 direction until at approximately  $H=0.14$  the lattice becomes saturated and the purple and brown spins become parallel to the field direction.

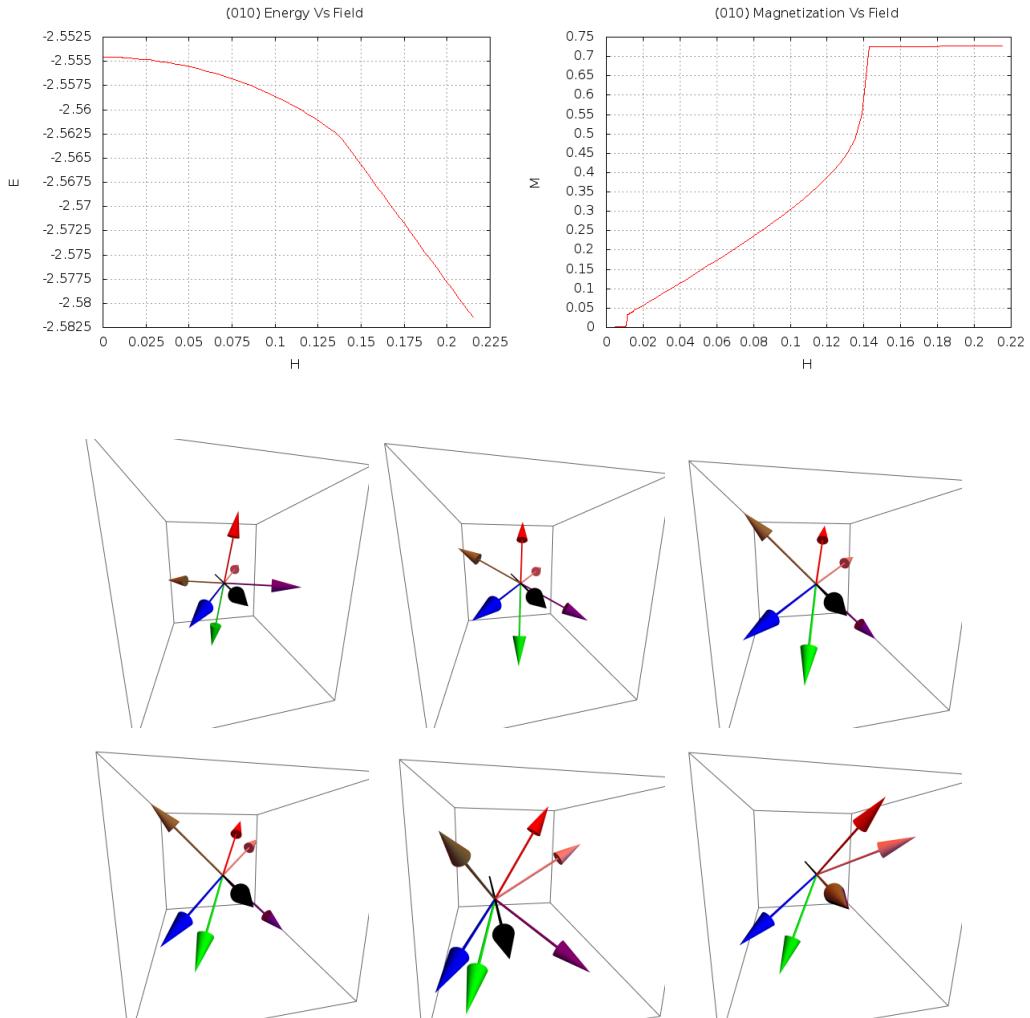


Figure 5: Snapshots at  $H=0, 0.0110, 0.0117, 0.0150, 0.139, 0.179$

## 5 (010) Decreasing Field, Ground State

The lattice is released from saturation at approximately field=0.13, a field magnitude lower than the increasing field required to induce saturation. The spins gradually unalign with the decreasing field, and rest at a zero field planar state characterized by angles theta=52.7 degrees and phi=-117.275 degrees.

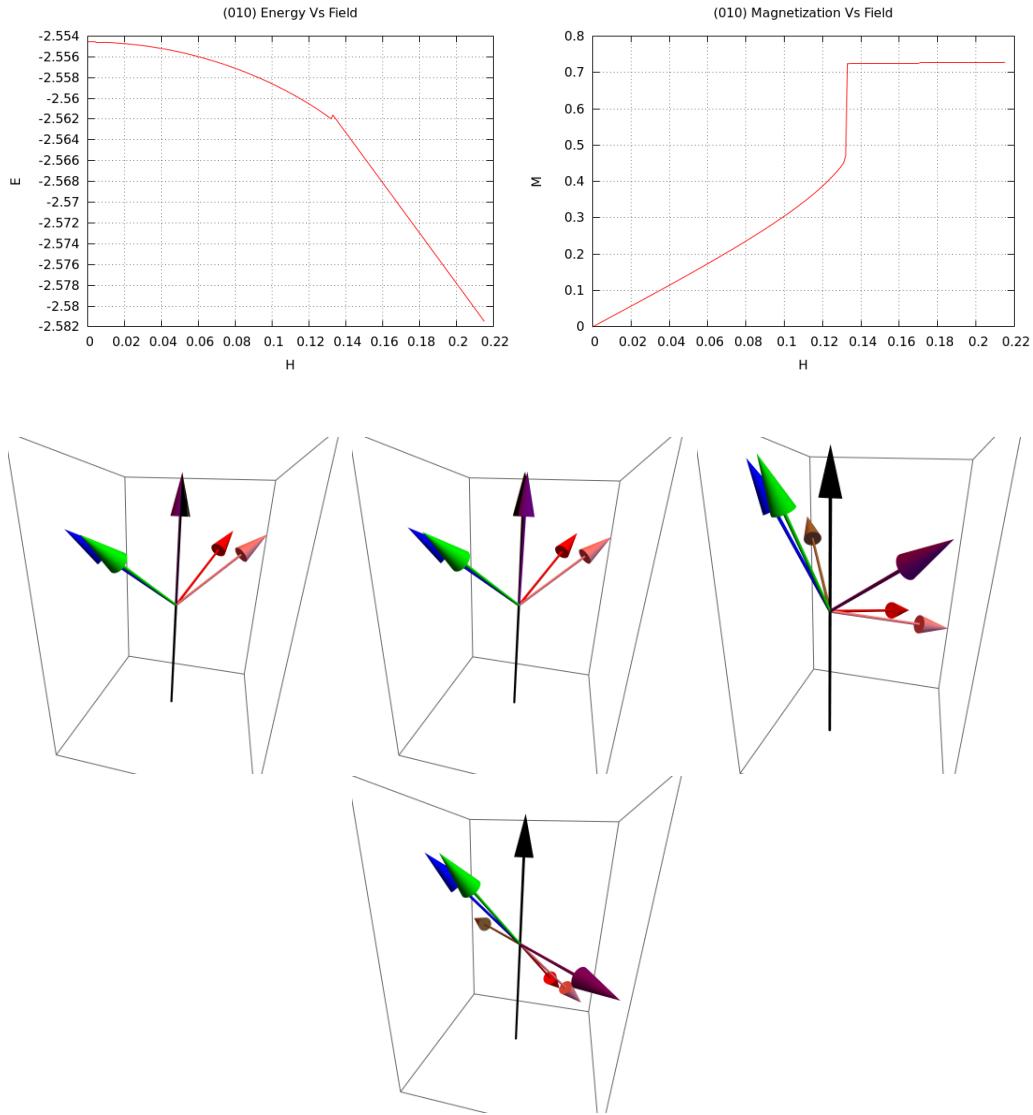


Figure 6: Snapshots of the 6 characteristic spins at  $H=0.215, 0.132, 0.131, 0$ . While the field arrow is pointing up, it is still pointing in the 010 direction.

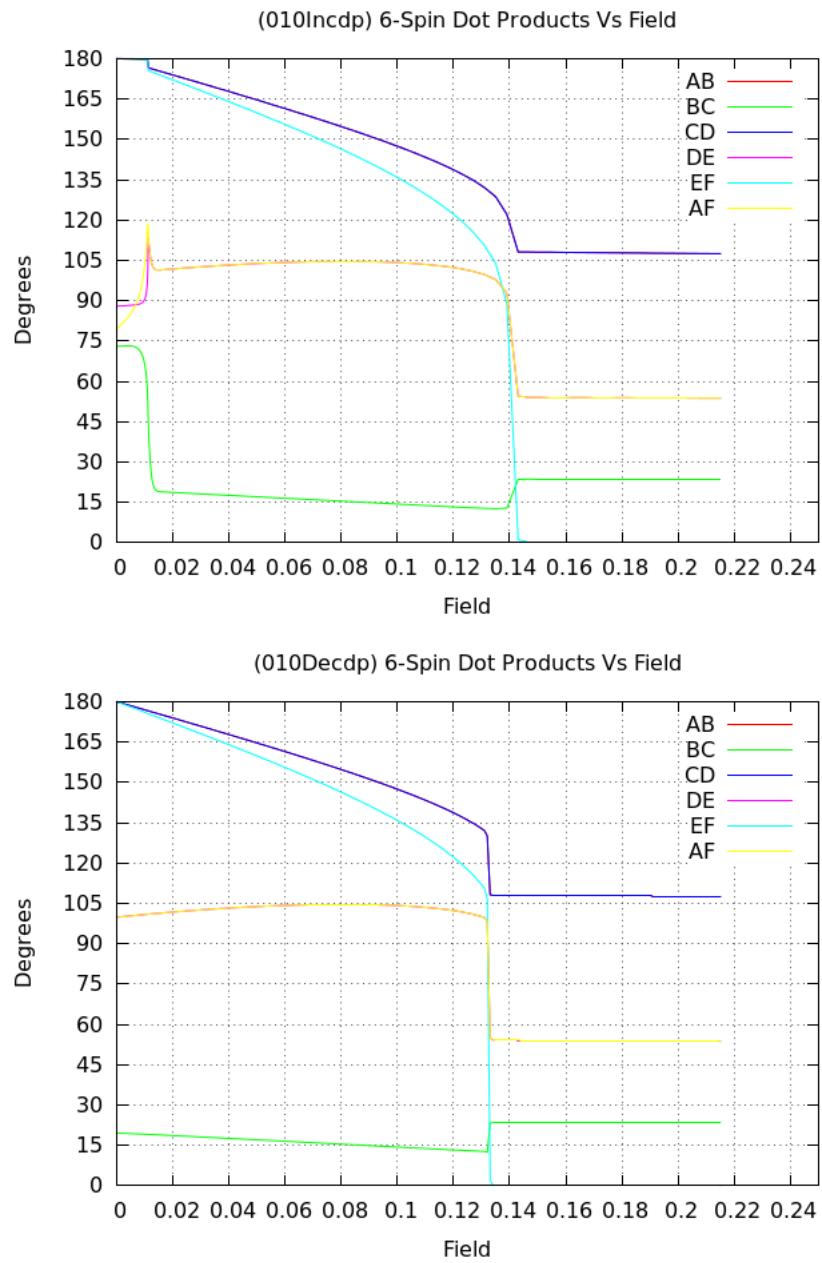


Figure 7: Dot products between the characteristic spins for both increasing and decreasing field.

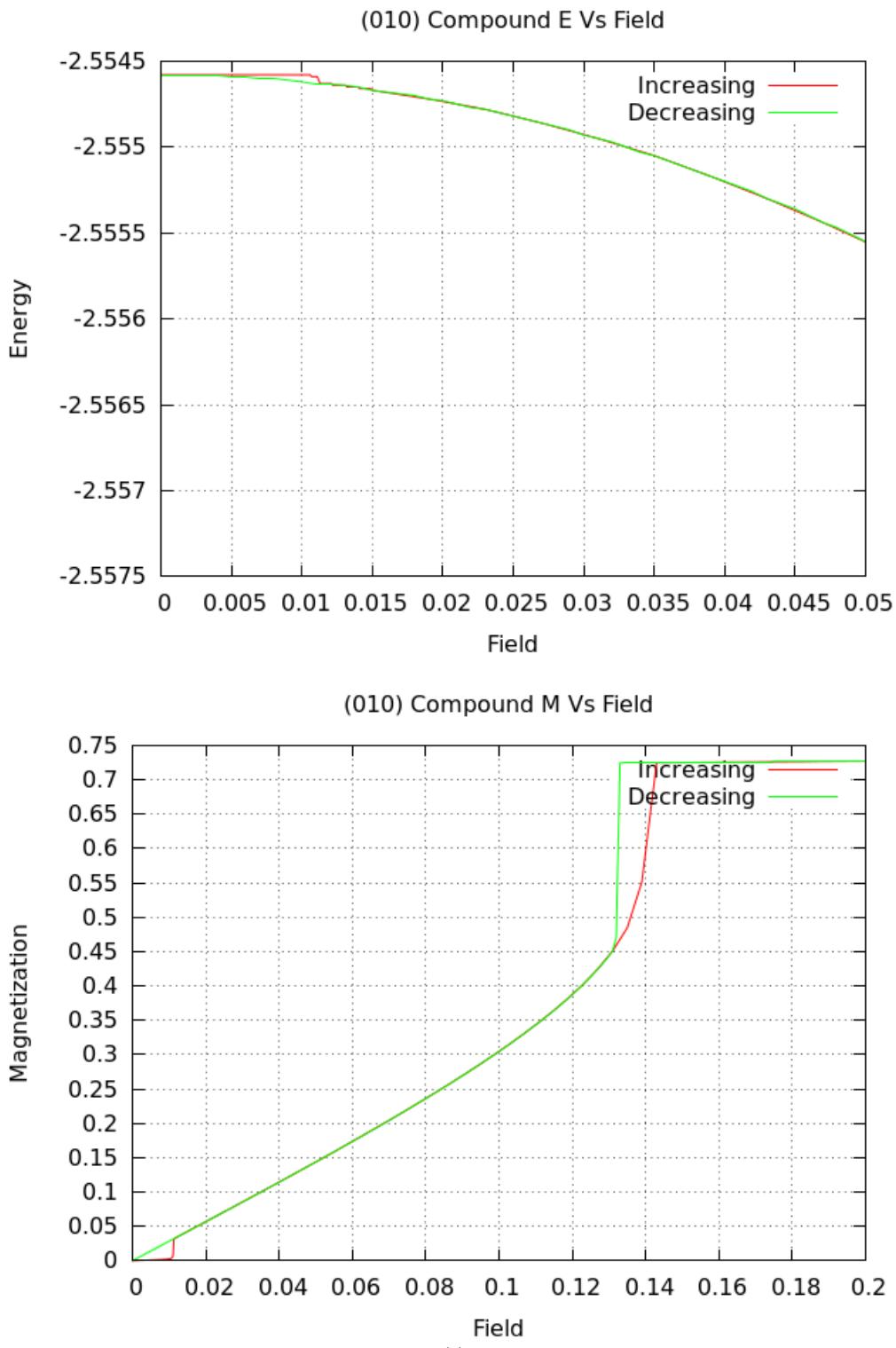


Figure 8: Composite graphs of energy and magnetization for both decreasing and increasing field magnitude.

## 6 (011) Increasing Field, Ground State

The lattice begins to transition at approximately 0.007. At 0.0074 the planar state is achieved. At 0.0093, the pink and red spins swap position, and the blue and green spins swap position. As the field is increased further to 0.0115, the green and brown spins begin to swap positions. At 0.143, this is achieved. Once saturated, no spins are parallel with the field direction.

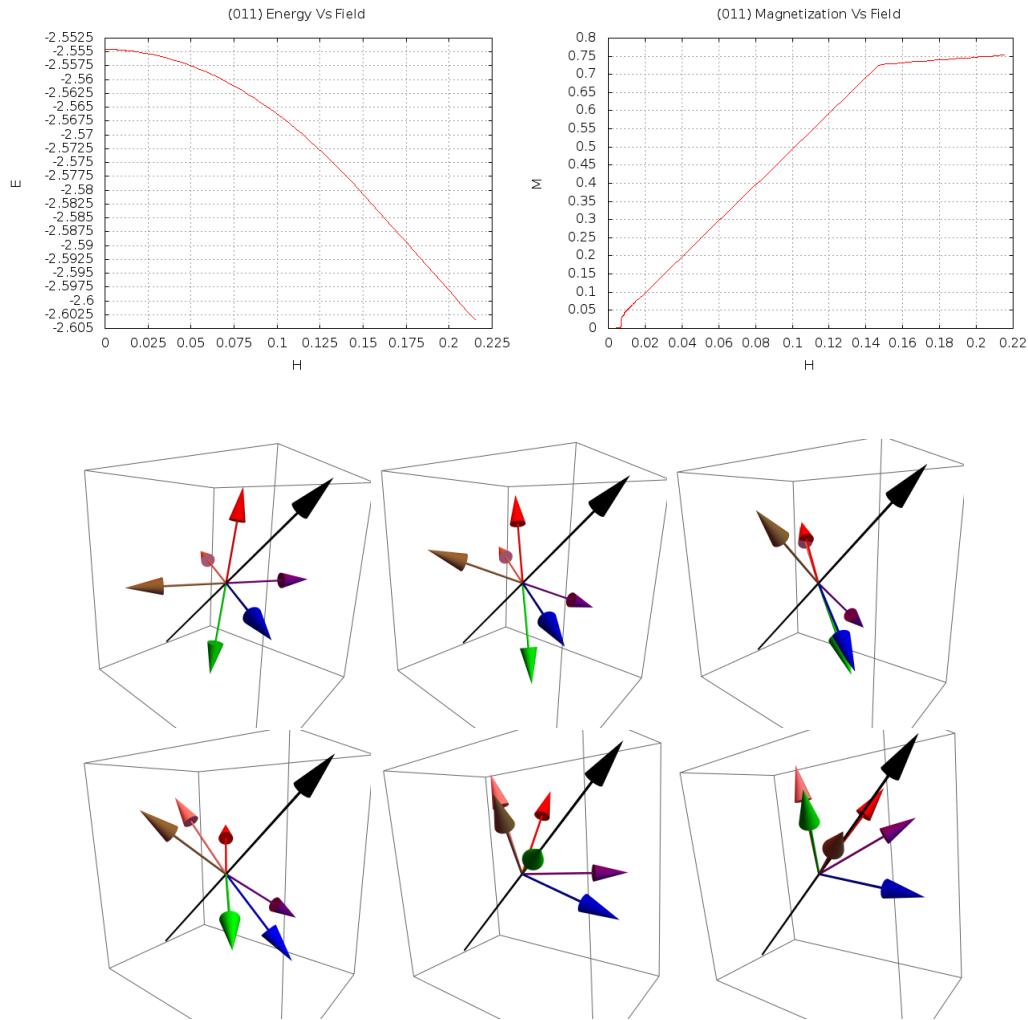


Figure 9: Snapshots at  $H=0, 0.0066, 0.0082, 0.0094, 0.115, 0.167$

## 7 (011) Decreasing Field, Ground State

As the field is decreased to 0.134, the brown and green spins swap positions again. All 6 spins gradually unalign with the field until they reach a zero field planar state characterized by angles theta=69.33 degrees and phi=-139.133 degrees.

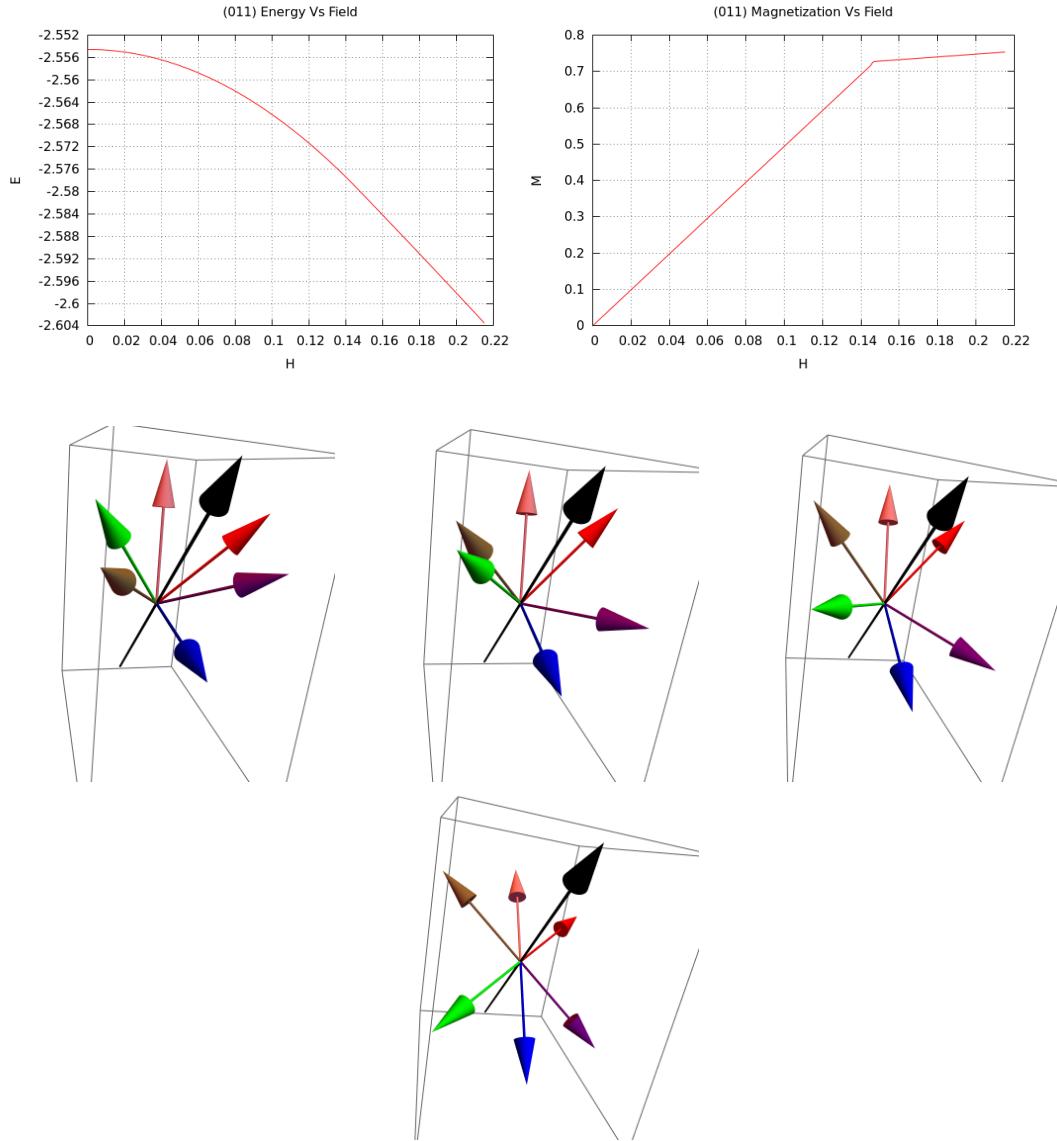


Figure 10: Snapshots at  $H=0.215, 0.134, 0.094, 0$

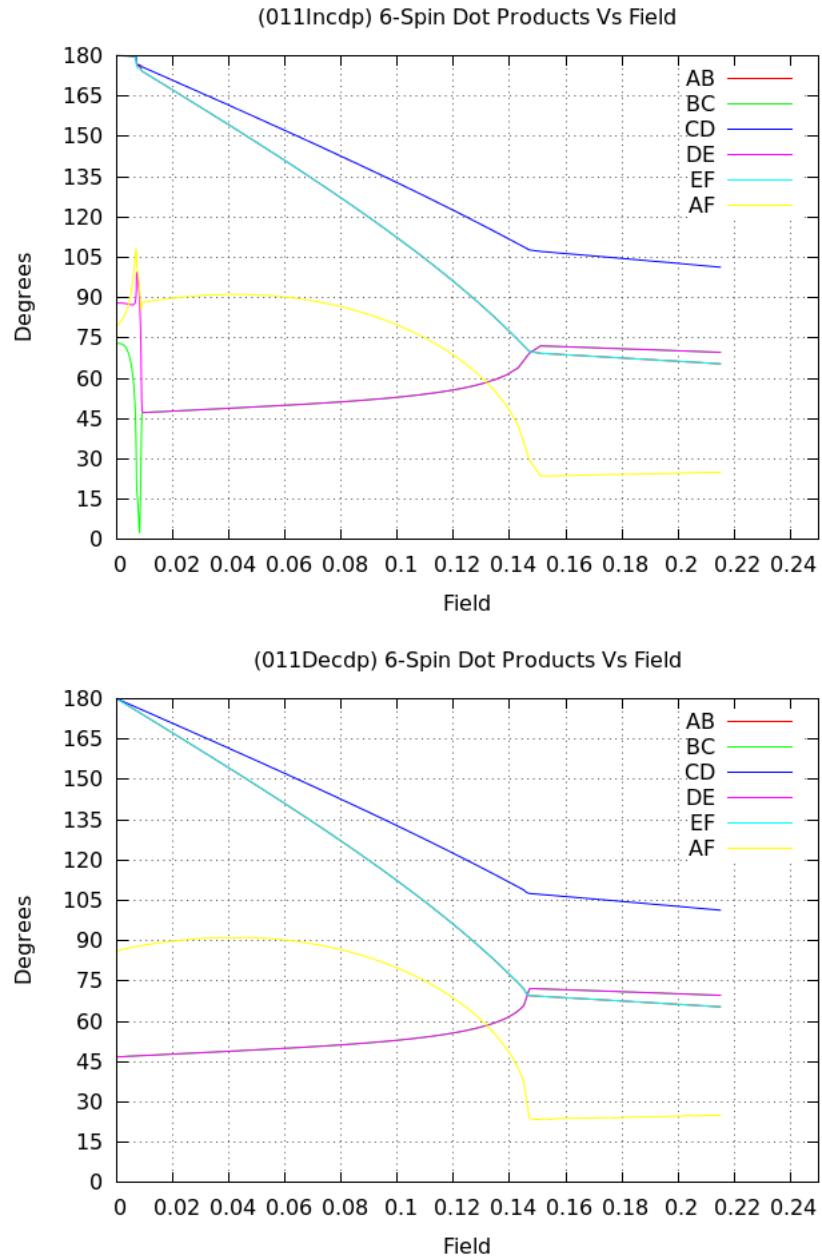


Figure 11: Dot products between the characteristic spins for both increasing and decreasing field.

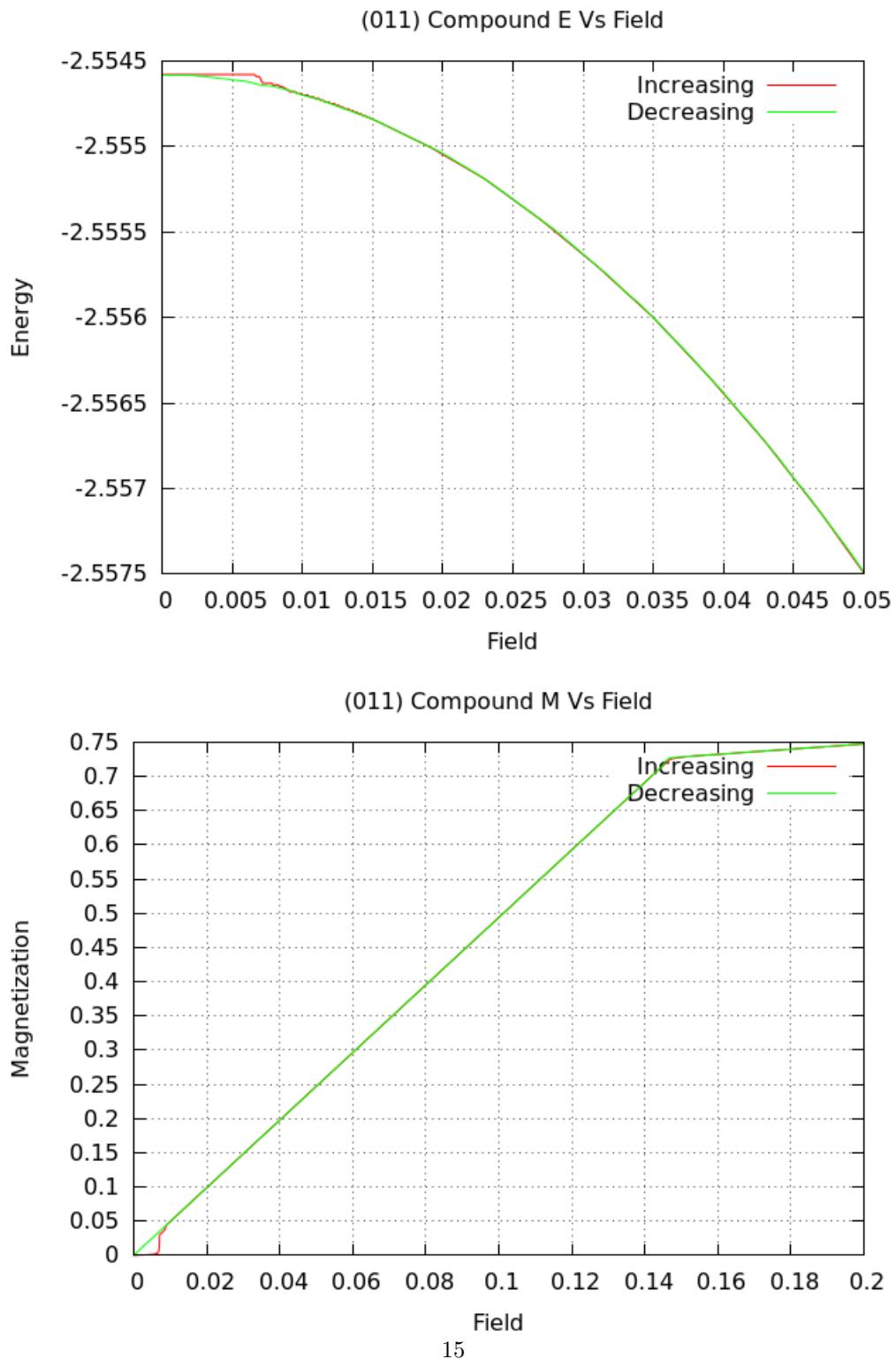


Figure 12: Composite graphs of energy and magnetization for both decreasing and increasing field magnitude.

## 8 (100) Increasing Field, Ground State

Two inflection points are observed in the magnetization graph. There are two inflection points in the energy graph as well, however they are not as obvious. A planar state is achieved at 0.0041. Between 0.0041 and 0.0064, the brown and green spins become closer to one another, as do the red and purple spins. The pink and blue spins remain fixed. The spins gradually align with the field, until it suddenly snaps into its final position where the blue and pink spins point in the same direction, in addition to lying within the xy plane. The lattice is saturated beyond this point.

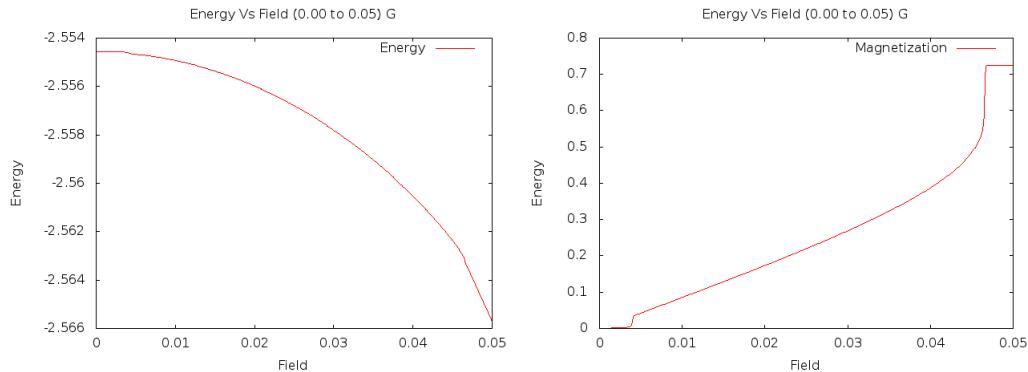


Figure 13: Energy vs increasing field and Magnetization versus increasing field

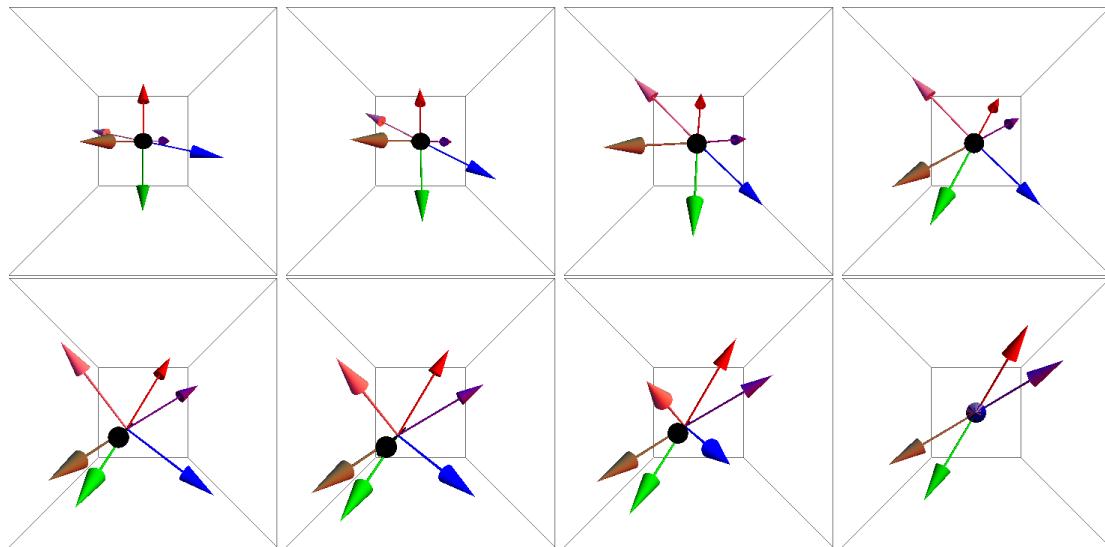


Figure 14:  $H=0, 0.0038, 0.0041, 0.0054, 0.0418, 0.0465, 0.0466$  and  $0.05$

## 9 (100) Decreasing Field, Ground State

As the field is decreased, the spins are released from the saturated state, and return to the typically observed planar state, that gradually unaligns with the field direction as the field is decreased. Finally, the spins return to a full planar state, and not the original zero field ground state. The starting configuration of this run was not the final configuration of the (100) Increasing Field, Ground State run, but the same zero field ground state that the (100) Increasing Field, Ground state started from. The final configuration is characterized by angles theta=51.63 degrees and phi=154.414 degrees.

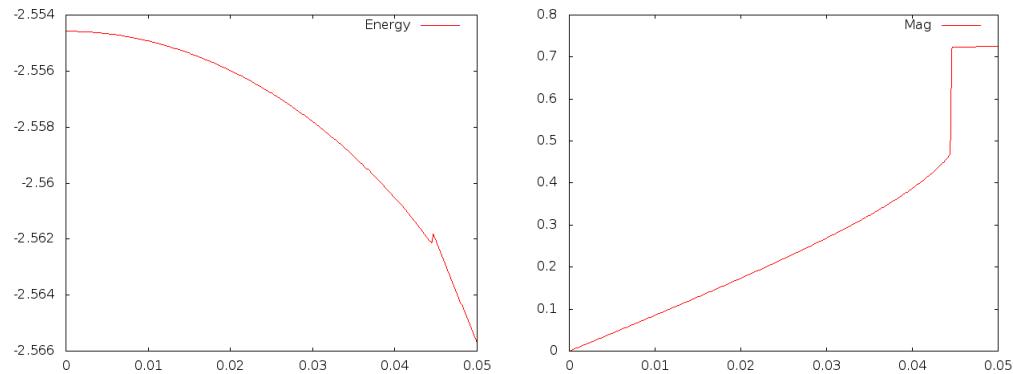


Figure 15: Energy vs decreasing field and Magnetization versus decreasing field

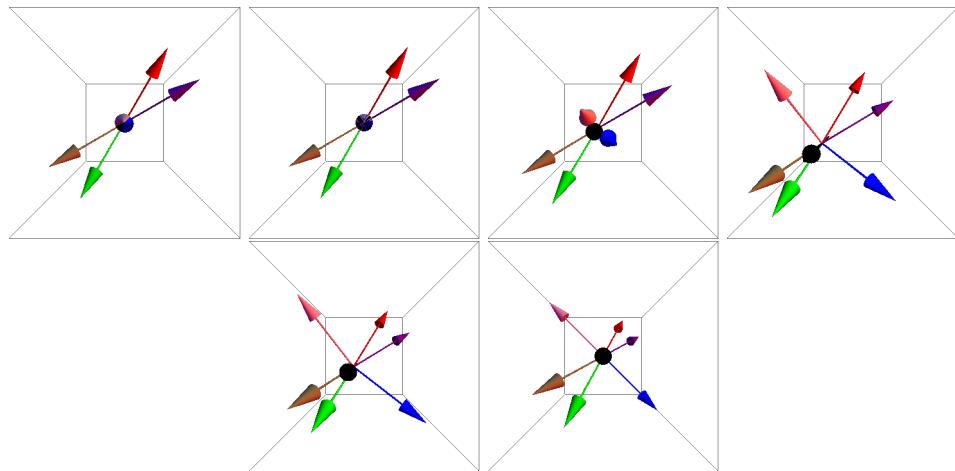


Figure 16:  $H=0.05, 0.0498, 0.0446, 0.0445, 0.0372$ , and  $0$ . It can be seen that the pink and blue spins have not yet entirely lined up with the field vector in the first picture, but they have in the second picture. This indicates that simply using a zero field groundstate and subjecting it to a high field immediately with only 3000 steps does not yield the true state for that field.

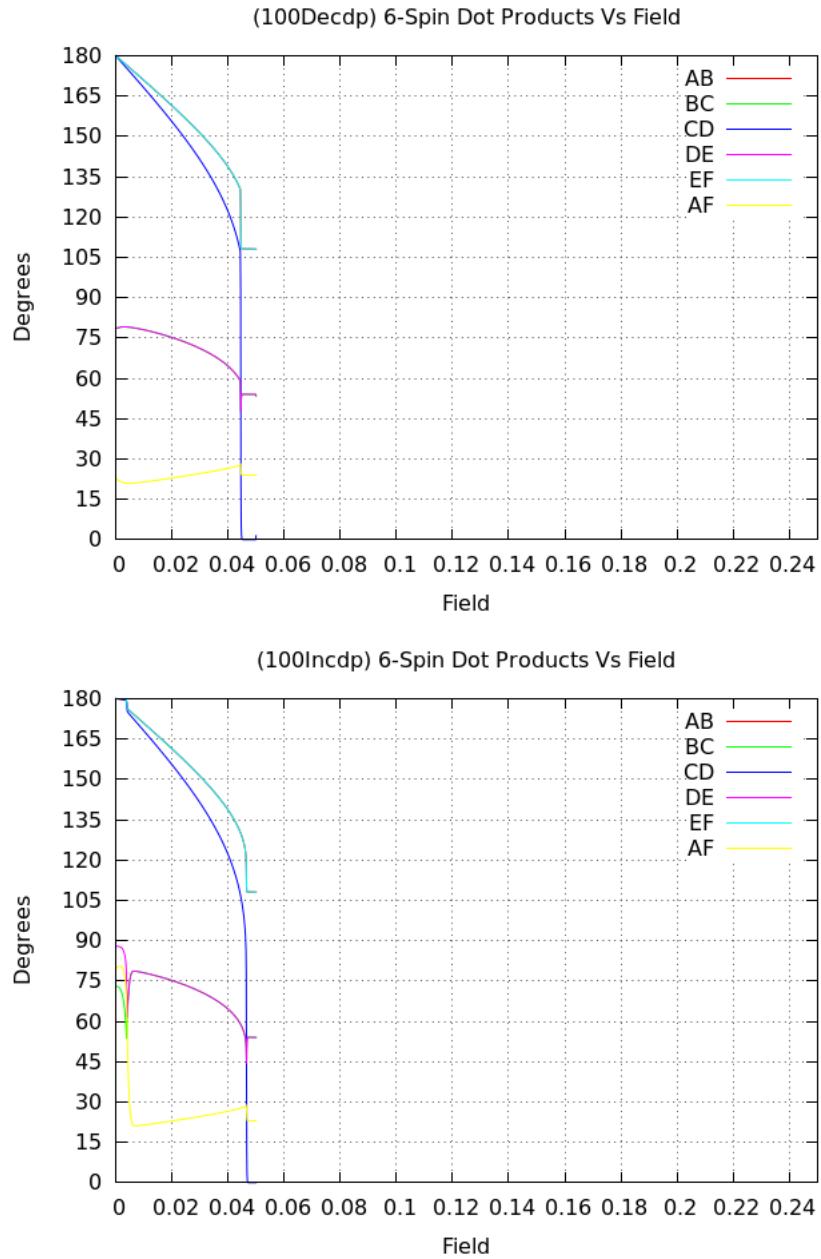


Figure 17: Dot products between the characteristic spins for both increasing and decreasing field. The data only continues to a low field relative to other simulations due to the saturation field occurring so early. A simulation continuing this run is currently being worked on.

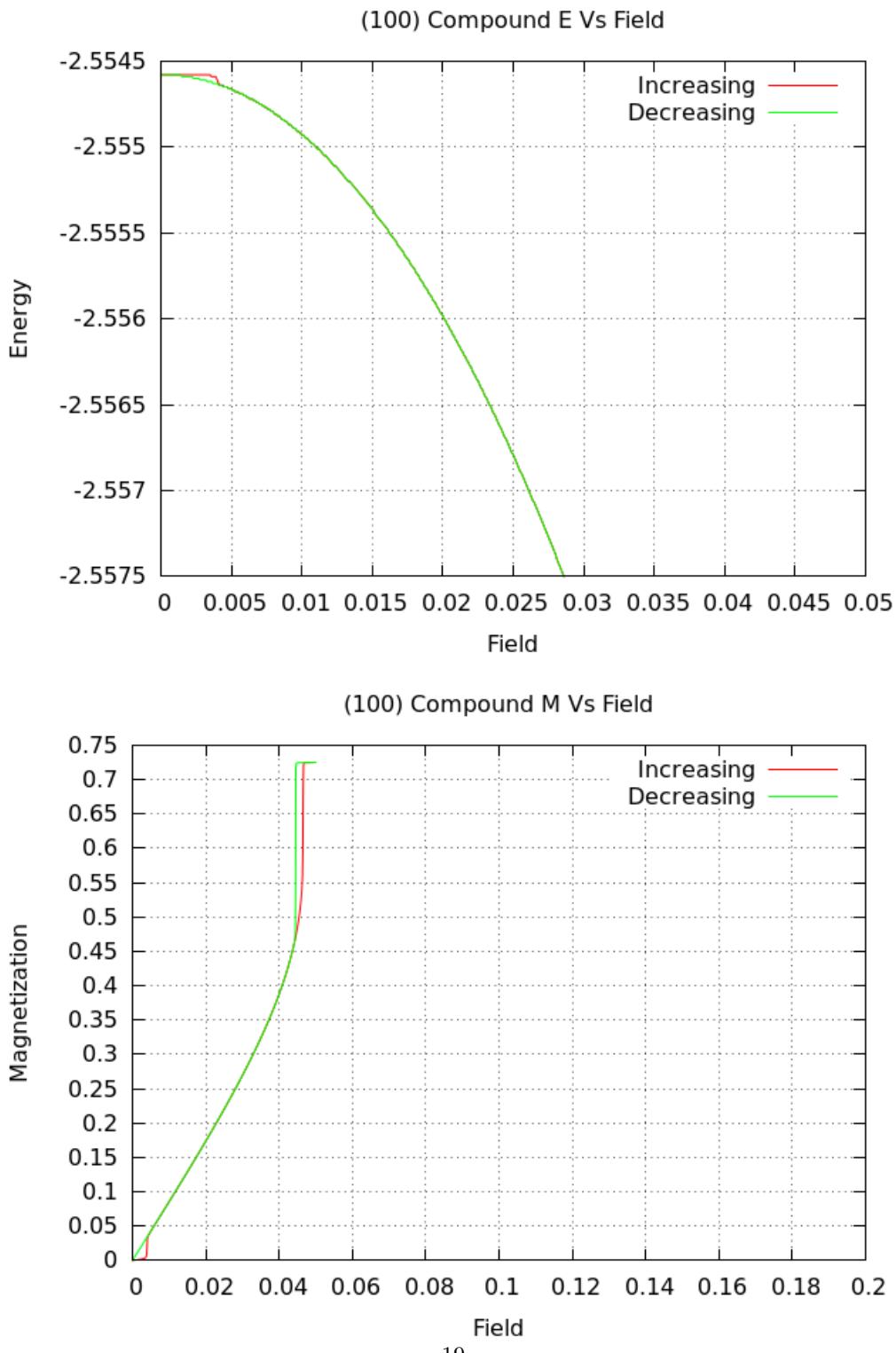


Figure 18: Composite graphs of energy and magnetization for both decreasing and increasing field magnitude.

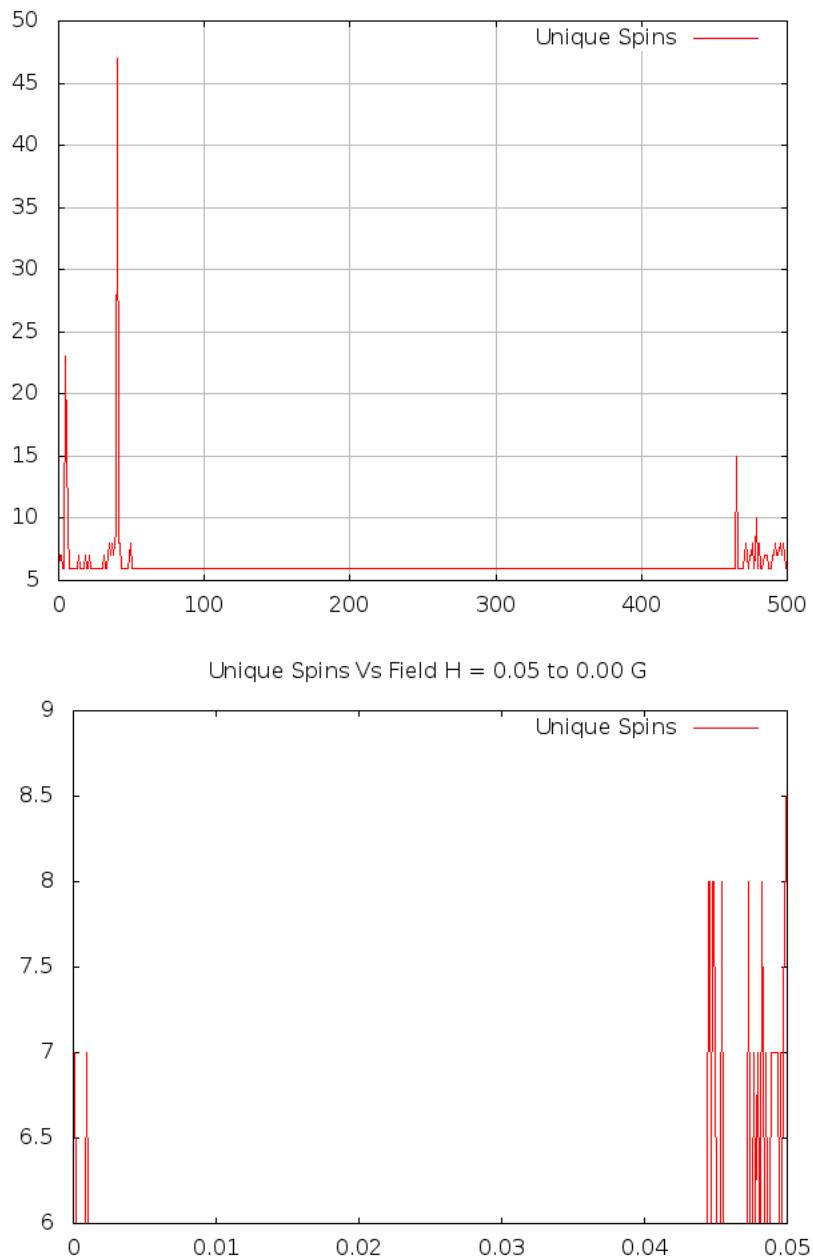


Figure 19: The number of unique spins within the lattice. The labelling is not clear, and not consistent throughout this pdf since these graphs were not completely finished at the time of making the pdf. The first graph's x axis begins at  $H=0$ , and ends at  $H=0.05$ , and depicts the number of spins within the system during an increasing field. The second is for decreasing field.

## 10 (100) Increasing Field, Random State

The energy drops very quickly at near zero field, which is likely because of insufficient number of iterations. Two points of inflection are observed. The transition of the spins is very similar to starting from a ground state.

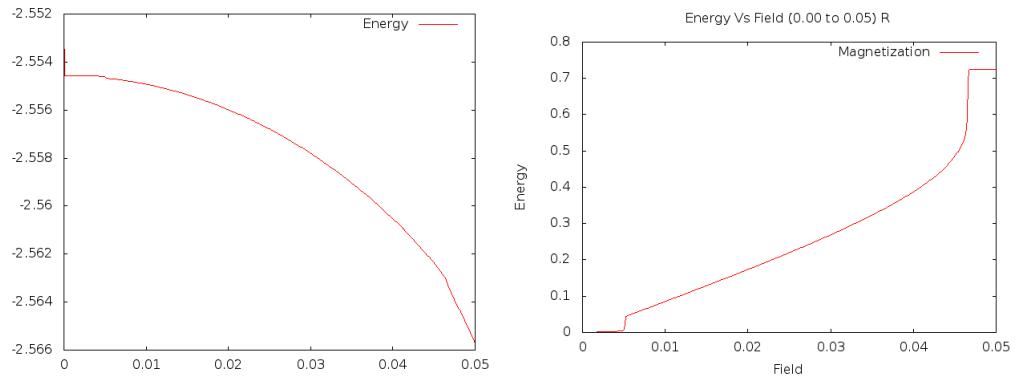


Figure 20: Energy vs increasing field and Magnetization versus increasing field

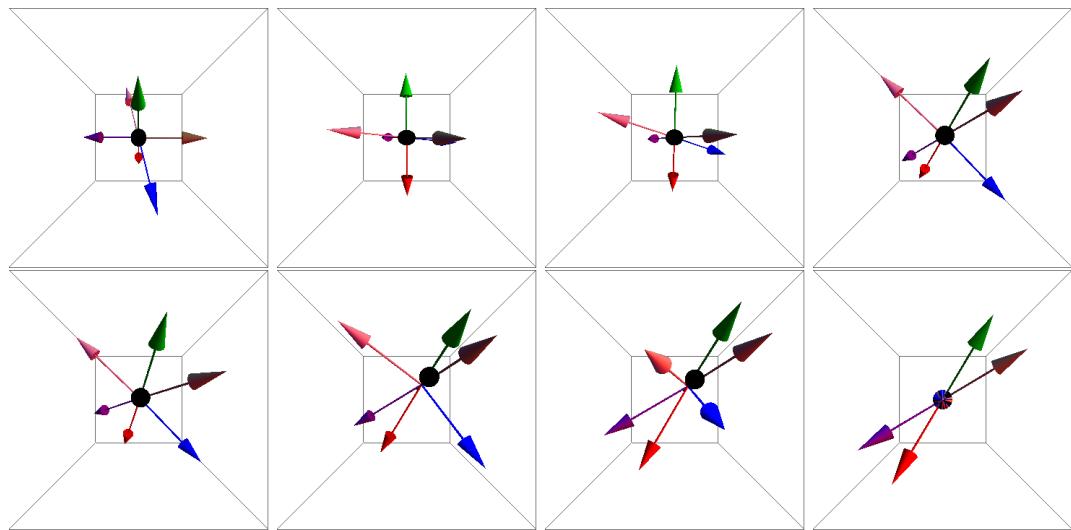


Figure 21:  $H = 0.00, 0.0001, 0.0047, 0.0053, 0.0054, 0.0410, 0.0466, 0.05$

## 11 (100) Decreasing Field, Random State

The lattice starts off in a planar state. As the field is decreased, spins gradually unalign with the field. Suddenly, at 0.0455, the spins snap back into a slight realigned planar state. Another sudden readjustment is observed at 0.025. Finally, the spins return a full planar state at 0 field. The red and brown spins swap positions as the field lowers, as do the green and purple spins. This is likely a result of insufficient EFM iterations.

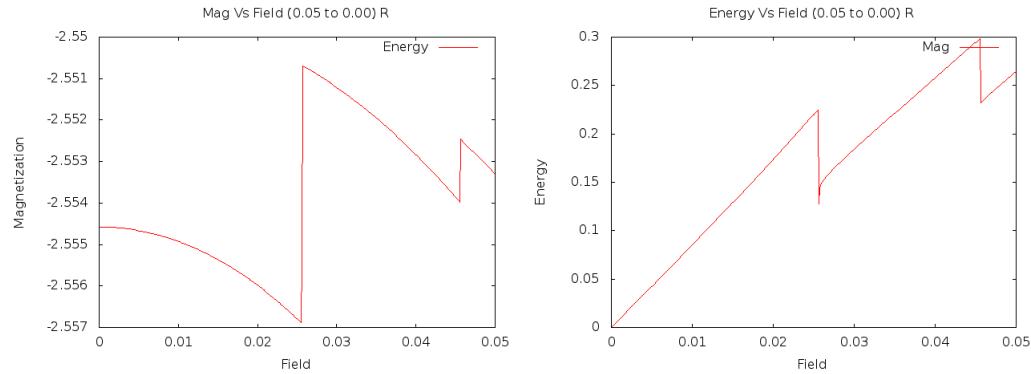


Figure 22: Energy vs decreasing field and Magnetization versus decreasing field

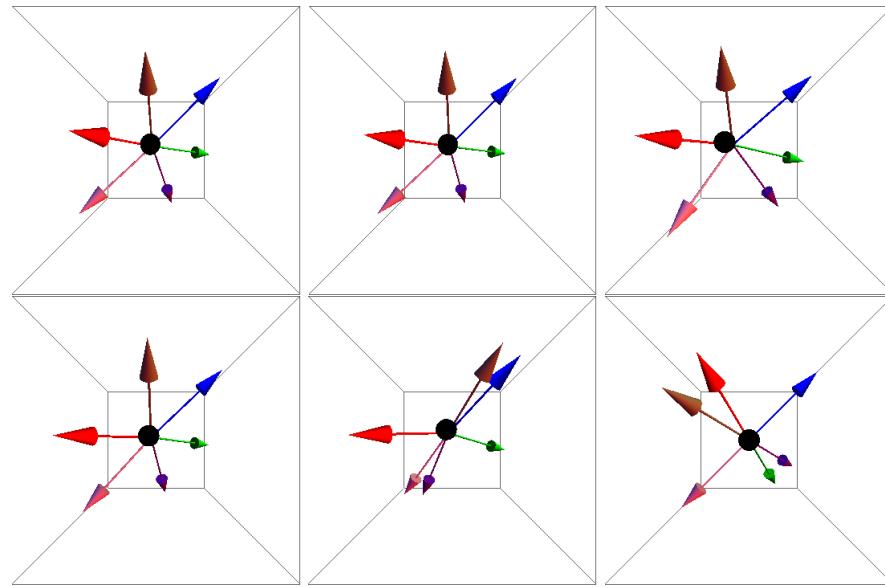


Figure 23:  $H = 0.05, 0.0460, 0.0455, 0.0257, 0.0256, 0.00$ .

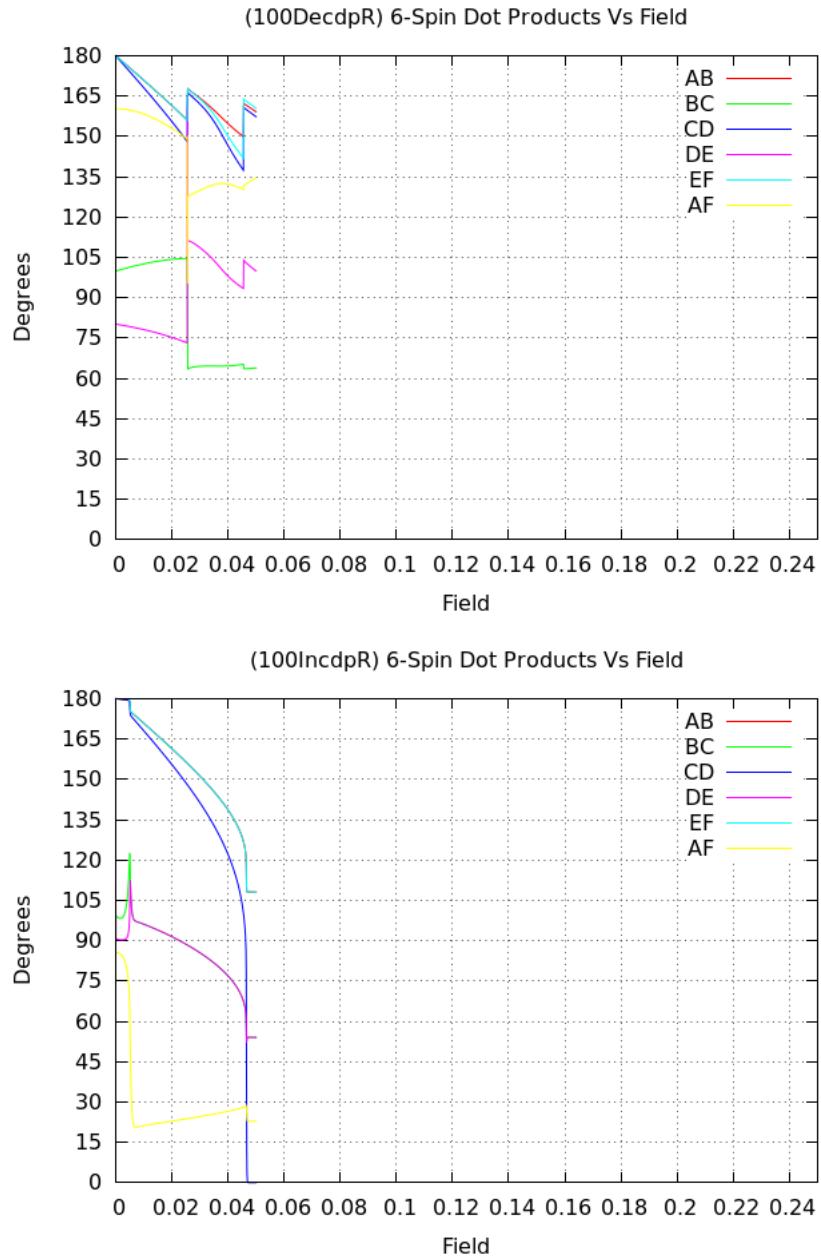


Figure 24: Dot products between the characteristic spins for both increasing and decreasing field. The data only continues to a low field relative to other simulations due to the saturation field occurring so early. A simulation continuing this run is currently being worked on.

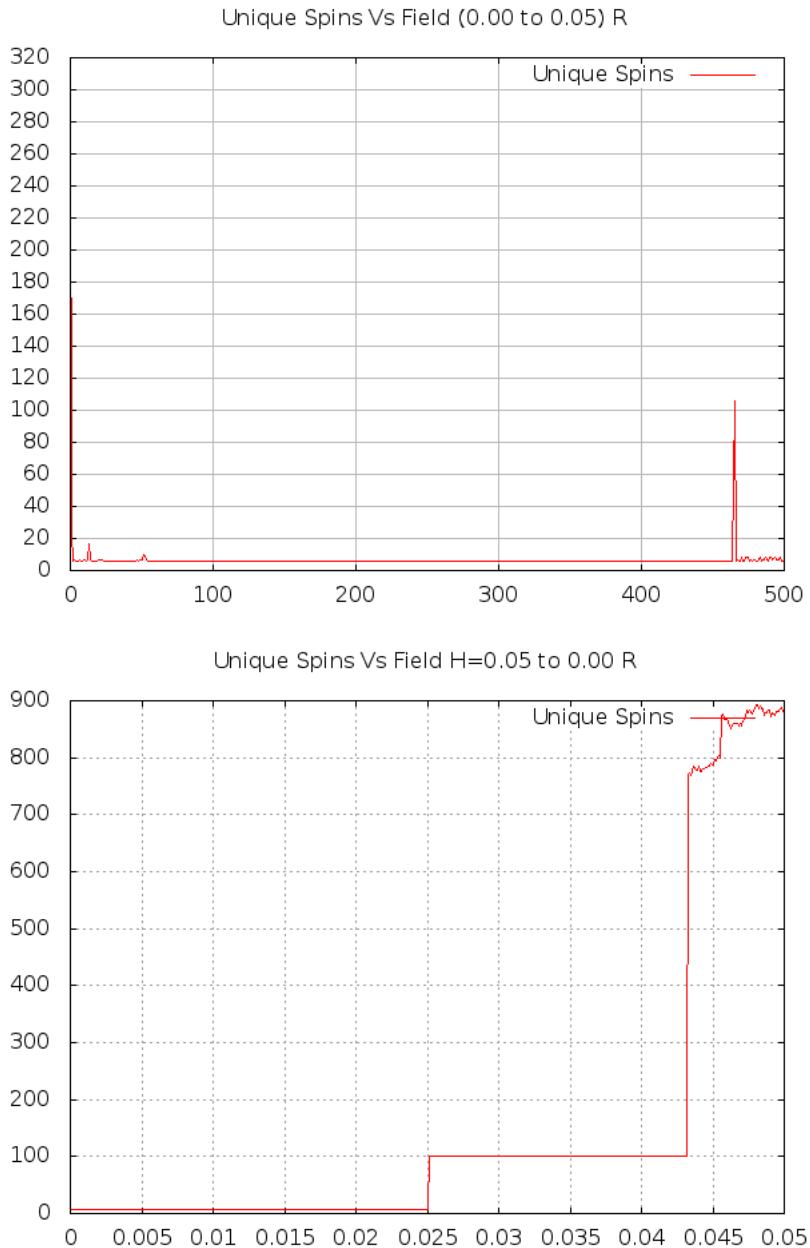


Figure 25: At high field, while decreasing it, a huge number of “*unique*” spins was observed. When looking through one of the configuration files, most spins only agreed with some other spins to at most 1 decimal place. The program that determines whether a spin is unique considers a spin to be unique when it doesn’t agree with any previously found spin up to at least two decimal places. Hence, the large number of unique spins present. The plateau in the middle is actually just false data I put into the text file, since I cancelled the program since it was taking a very long time. I reran the program from around  $H = 0.0250$  to 0, and found that the lattice in this field range always had 6 unique spins.

## 12 (101) Increasing Field, Ground State

The lattice begins to undergo a transition to a planar state at 0.0055, where it is achieved at 0.0060. At 0.0115 the purple and red spins and green and brown spins begin to swap positions, which is complete at 0.0128. At approximately 0.14, the green and pink spins swap position. Upon swapping, the lattice becomes saturated.

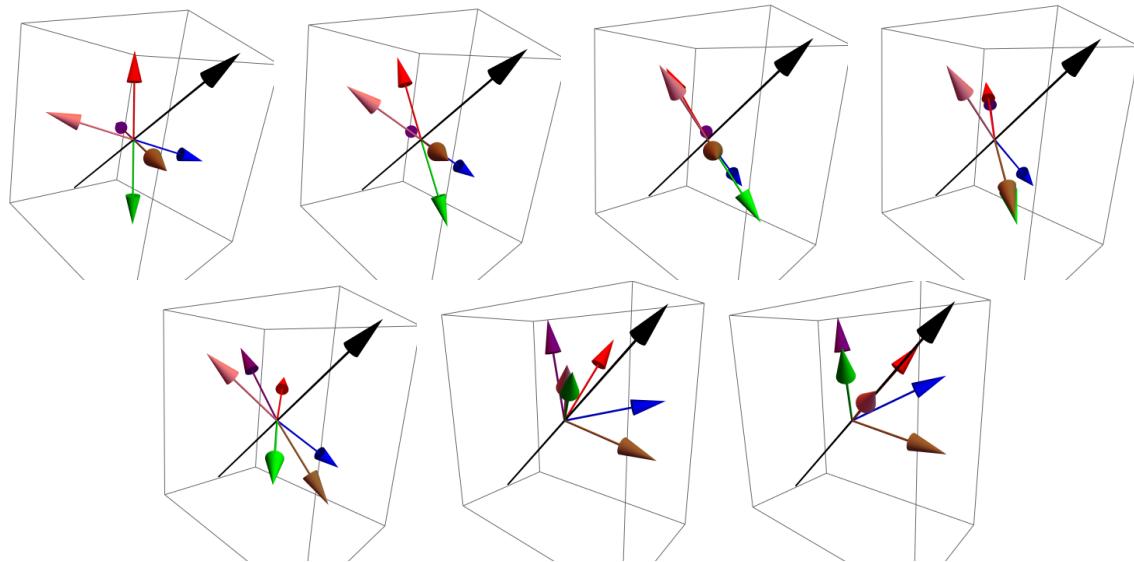
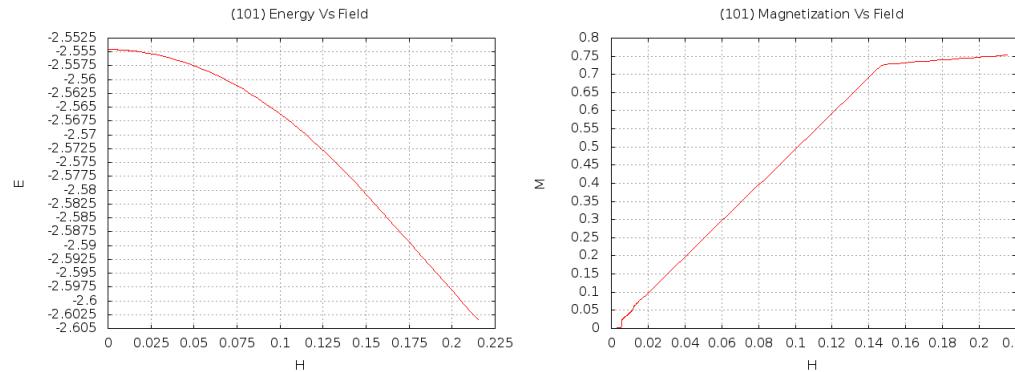


Figure 26: H=0, 0.0055, 0.0060, 0.0115, 0.0128, 0.0139, 0.163

## 13 (101) Decreasing Field, Ground State

When decreasing the field, instead of the pink and green re-swapping positions the blue and red spins, the spins that mirror them, swap positions at approximately 0.137. The final configuration is characterized by angles theta=110.826 degrees and phi=49.1513 degrees.

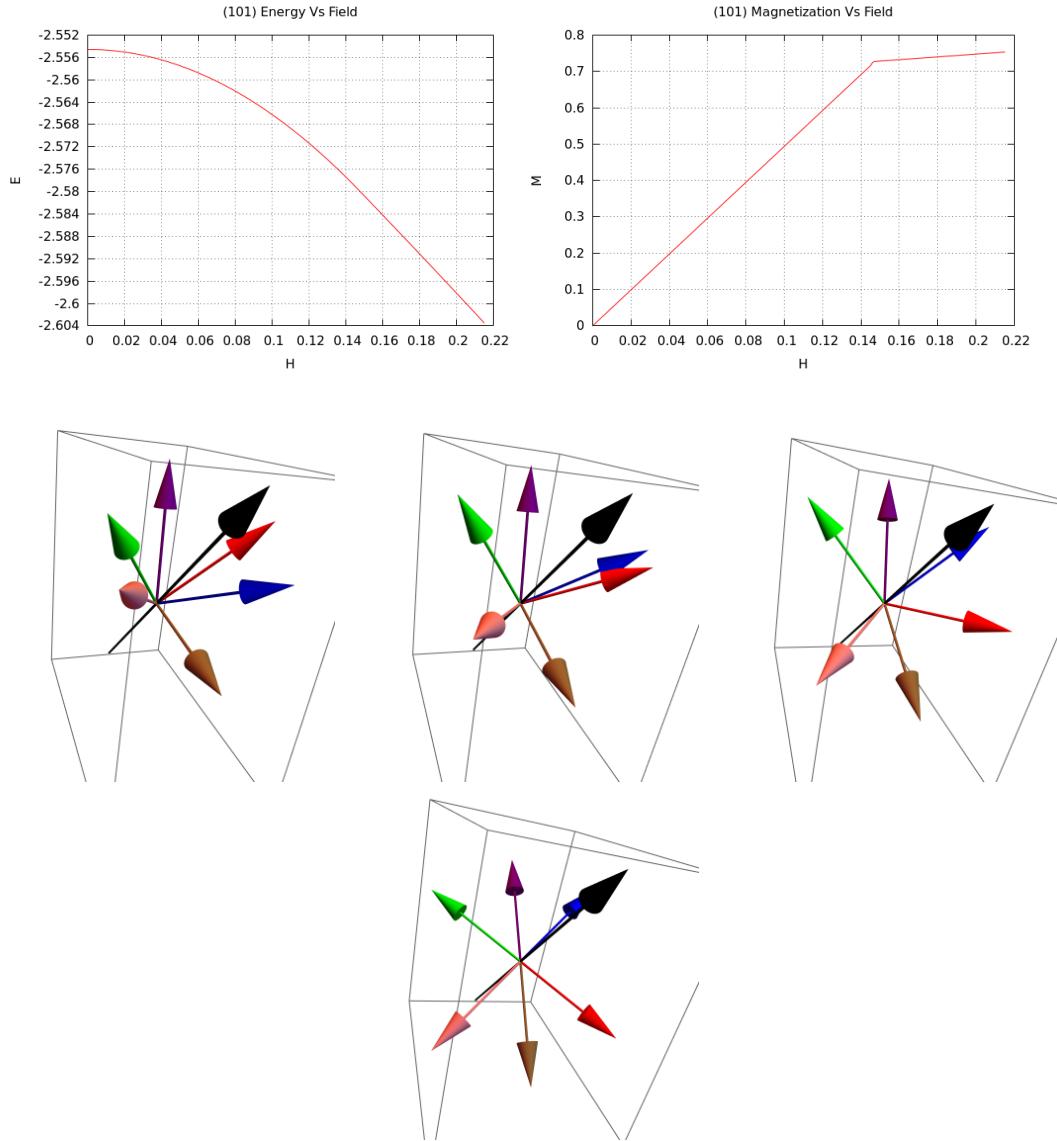


Figure 27: Snapshots at  $H=0.2150, 0.137, 0.09, 0$

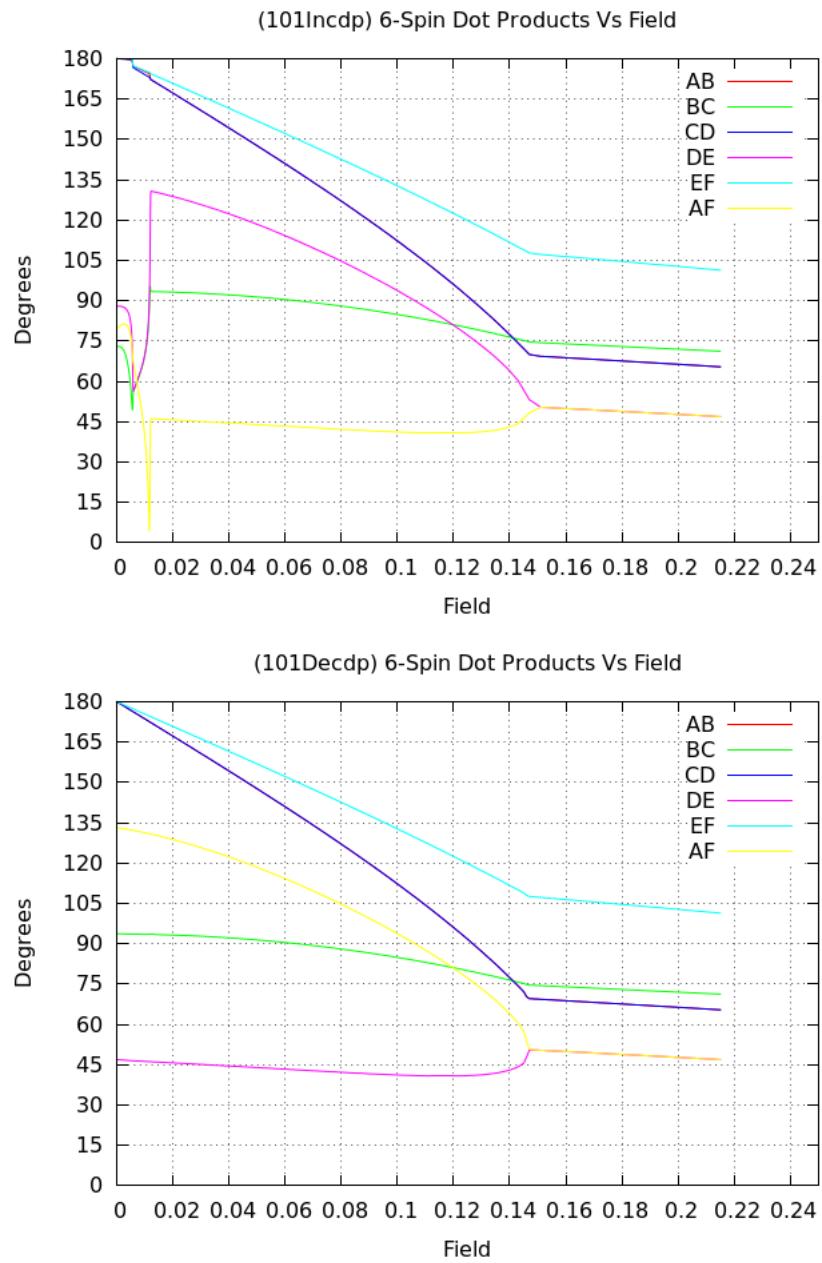


Figure 28: Dot products between the characteristic spins for both increasing and decreasing field.

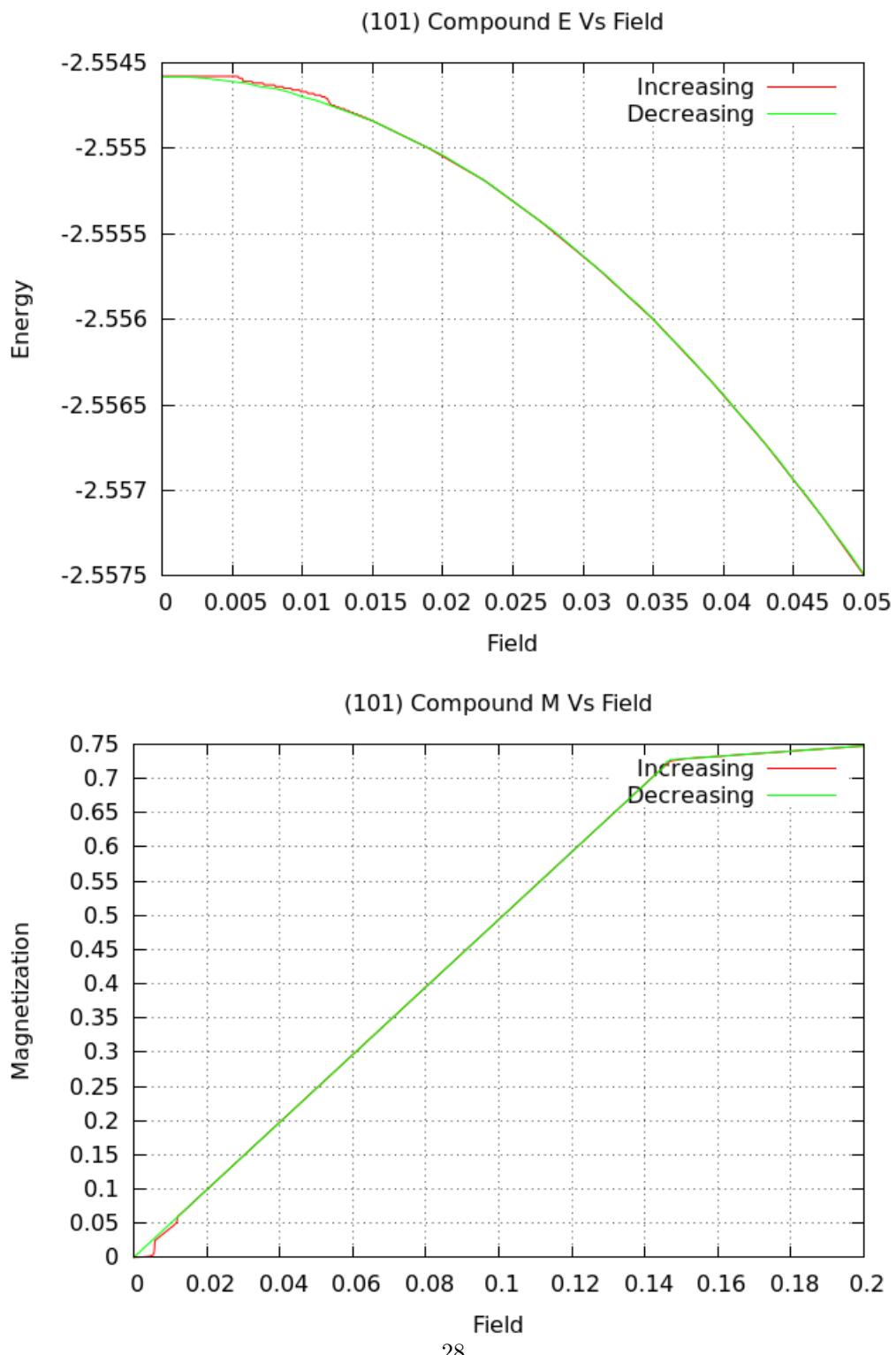


Figure 29: Composite graphs of energy and magnetization for both decreasing and increasing field magnitude.

## 14 (110) Increasing Field, Ground State

Two inflection points are evident in the graphs of energy and magnetization, indicating the occurrence 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. This is the result of the red and purple spins swapping positions, and the brown and green spins swapping positions.

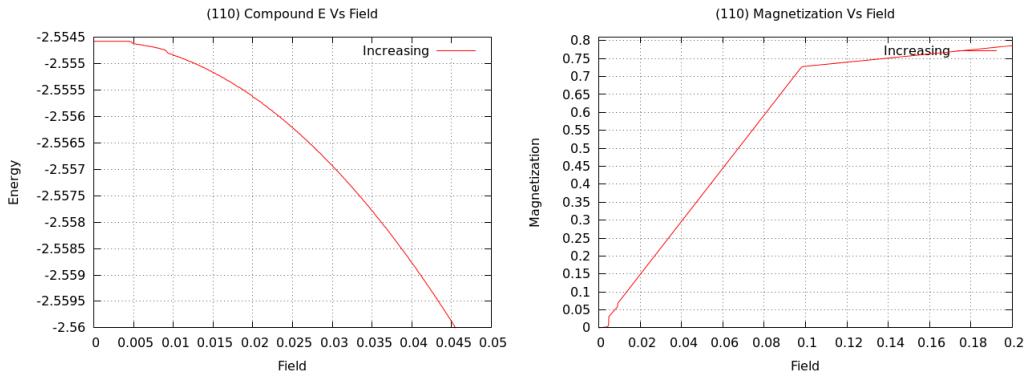


Figure 30: Energy vs increasing field and Magnetization versus increasing field

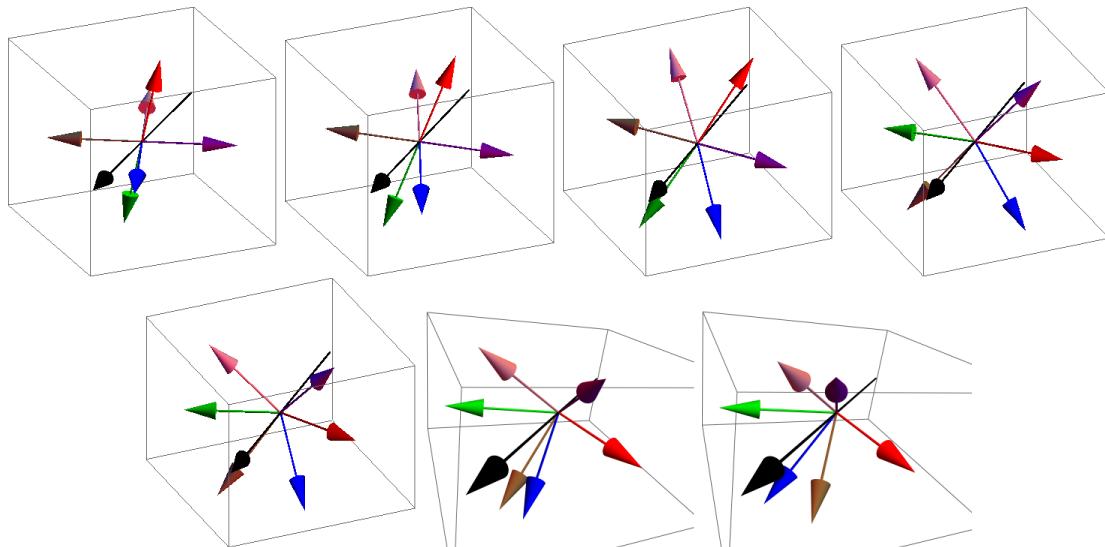


Figure 31: Snapshots of the 6 characteristic spins of the lattice at  $H=0$ , 0.0046, 0.0049, 0.0095, 0.05, 0.089, and 0.1

## 15 (110) 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. The final configuration has characteristic angles theta=90.096 degrees and phi=135.034 degrees. The starting configuration of this run was not the final configuration of the (110) Increasing Field, Ground State run, but the same zero field ground state that the (110) Increasing Field, Ground state started from.

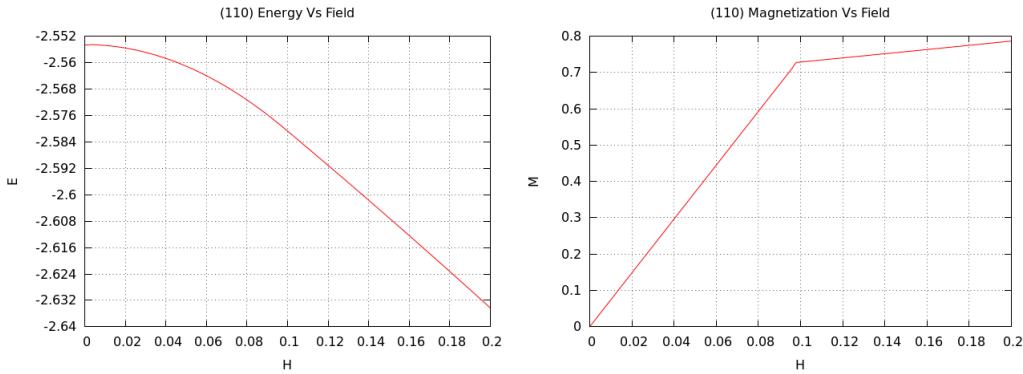


Figure 32: Energy vs decreasing field and Magnetization versus decreasing field

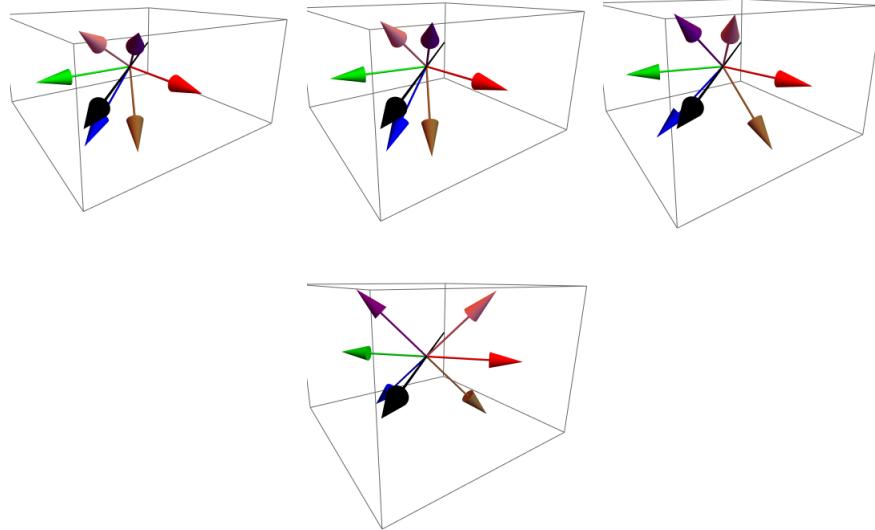


Figure 33: Snapshots of the 6 characteristic spins of the lattice at  $H=0.2, 0.121, 0.101$ , and 0

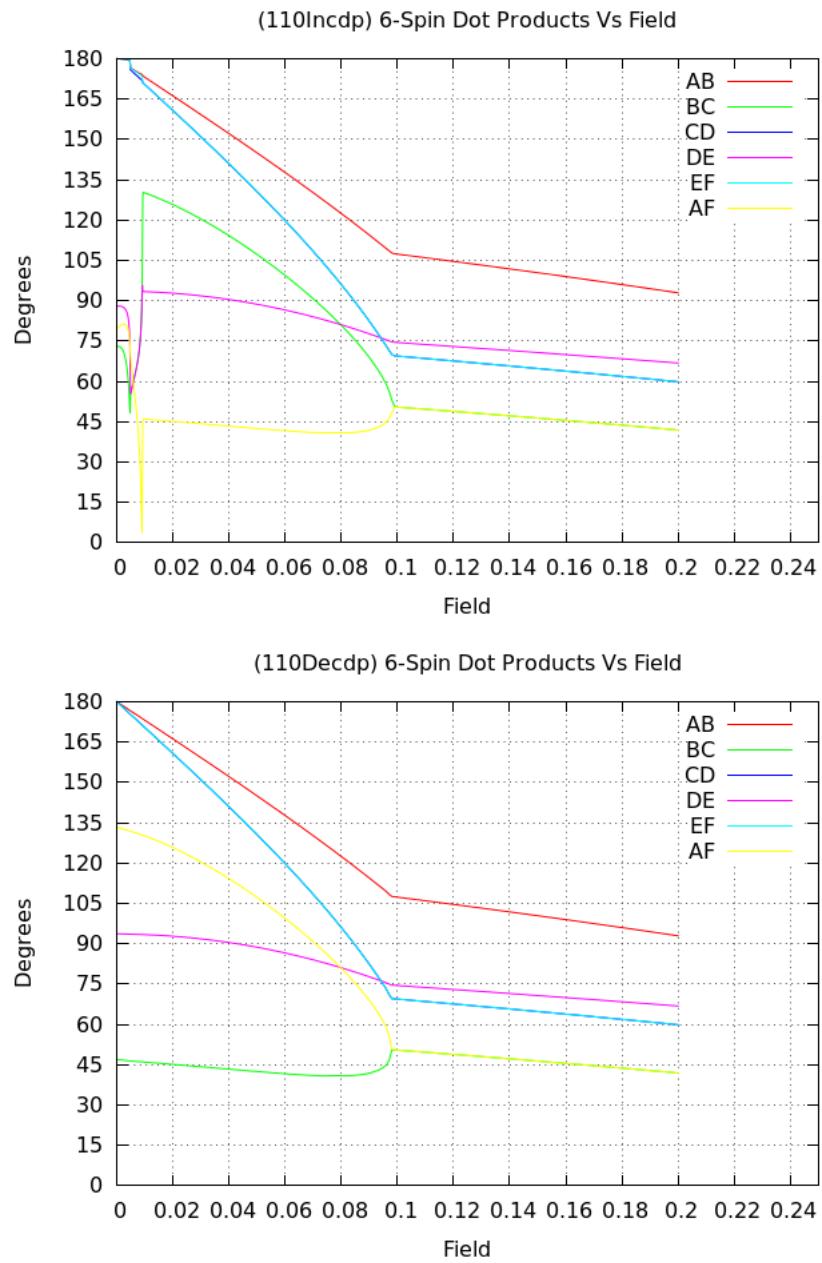


Figure 34: Dot products between the 6 characteristic spins of the lattice.

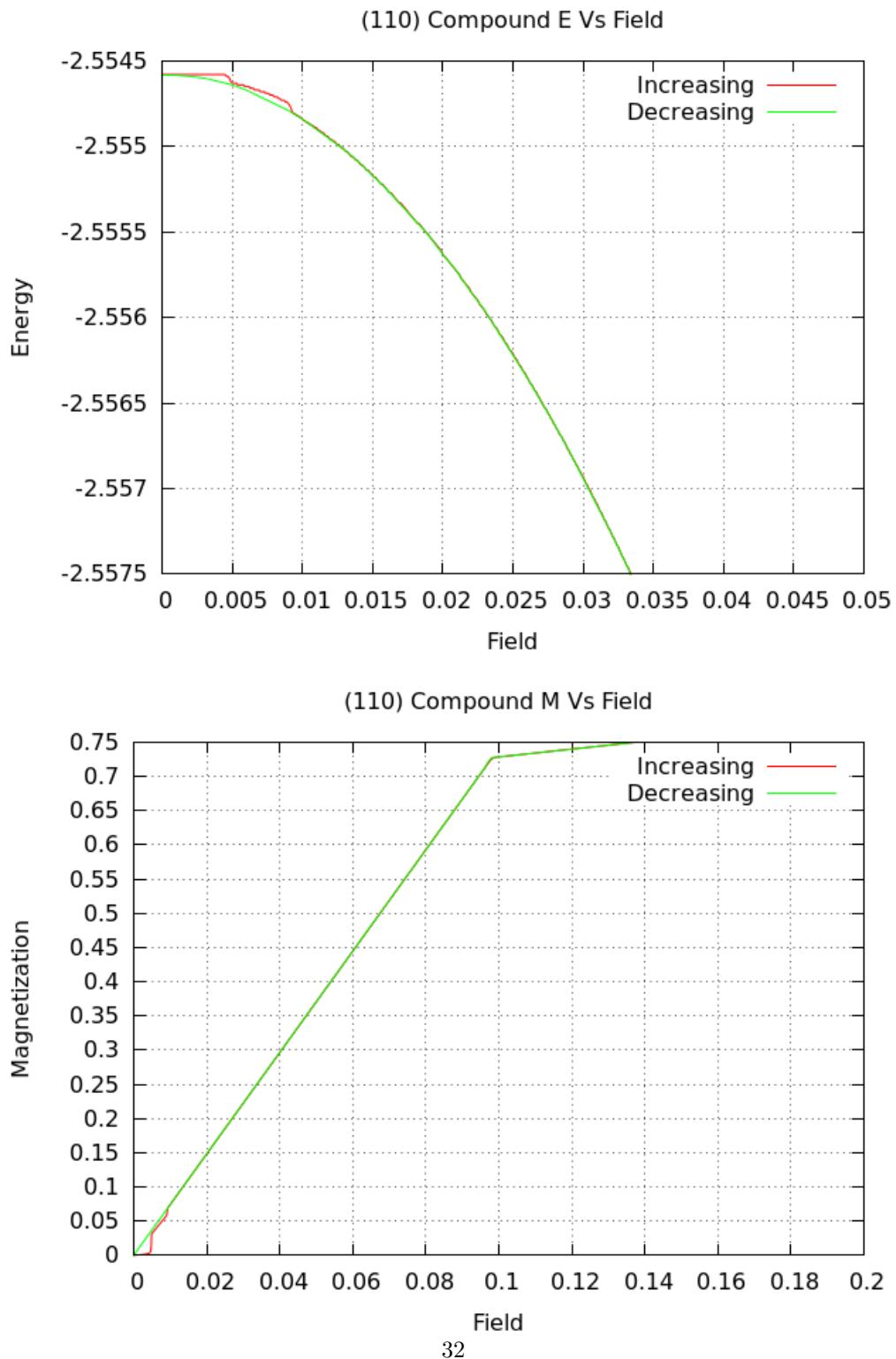


Figure 35: Composite graphs of energy and magnetization for both decreasing and increasing field magnitude.

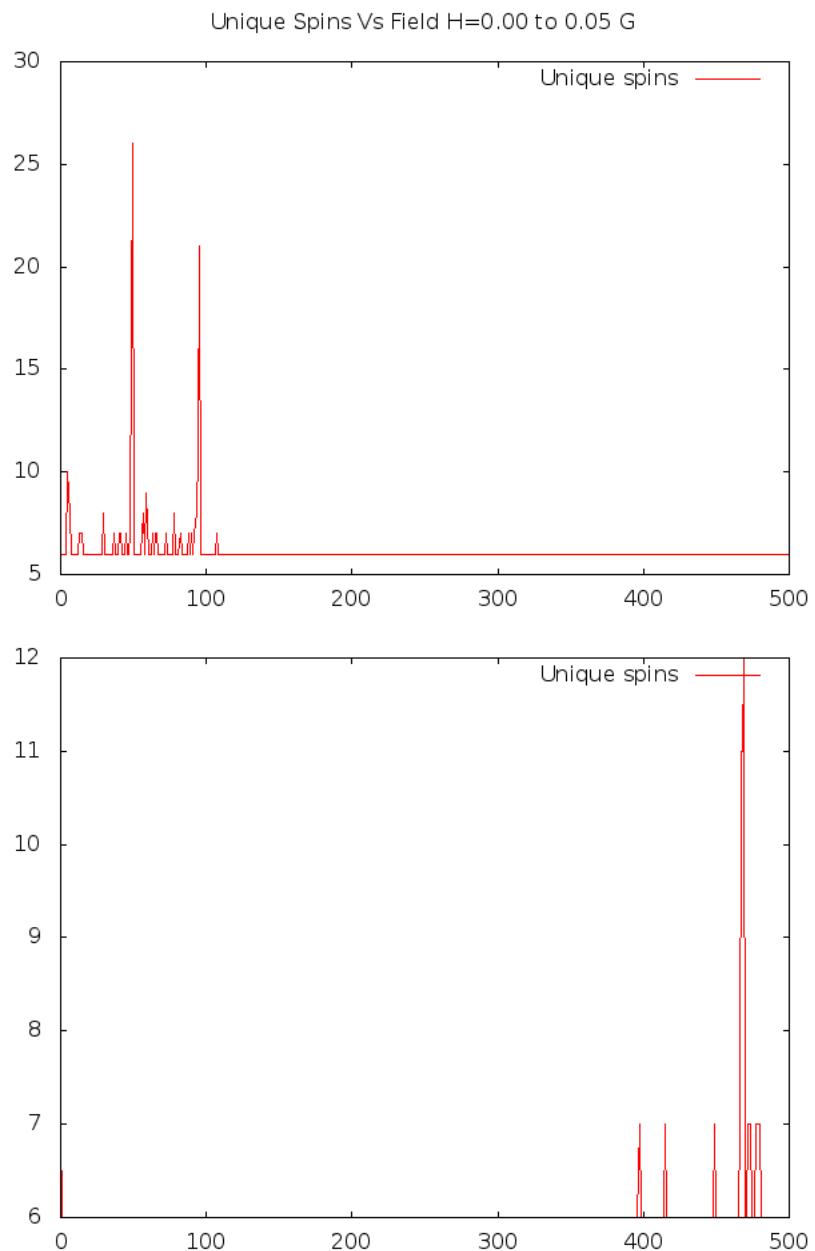


Figure 36: As mentioned before, these graphs aren't finished. The top graph's x-axis begins at  $H=0$ , and ends at  $H=0.05$ . The bottom graph's x-axis begins at  $H=0.05$  and ends at  $H=0$ .

## 16 (110) Increasing Field, Random State

Very similar to beginning with the ground state, 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.

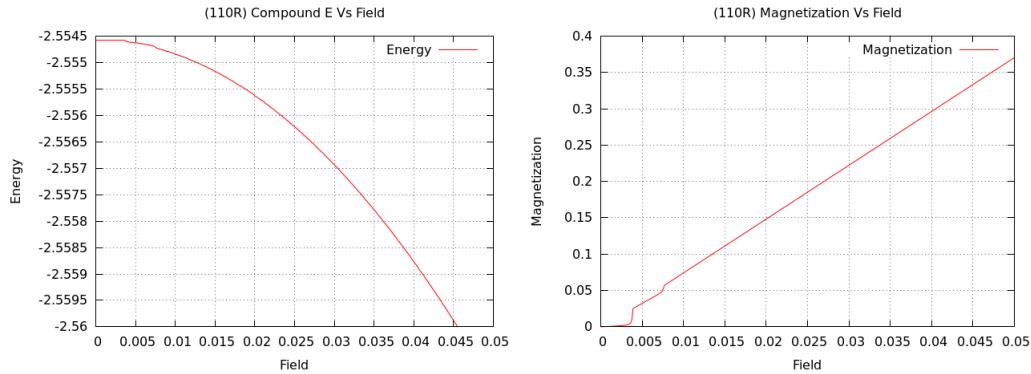


Figure 37: Energy vs increasing field and Magnetization versus increasing field

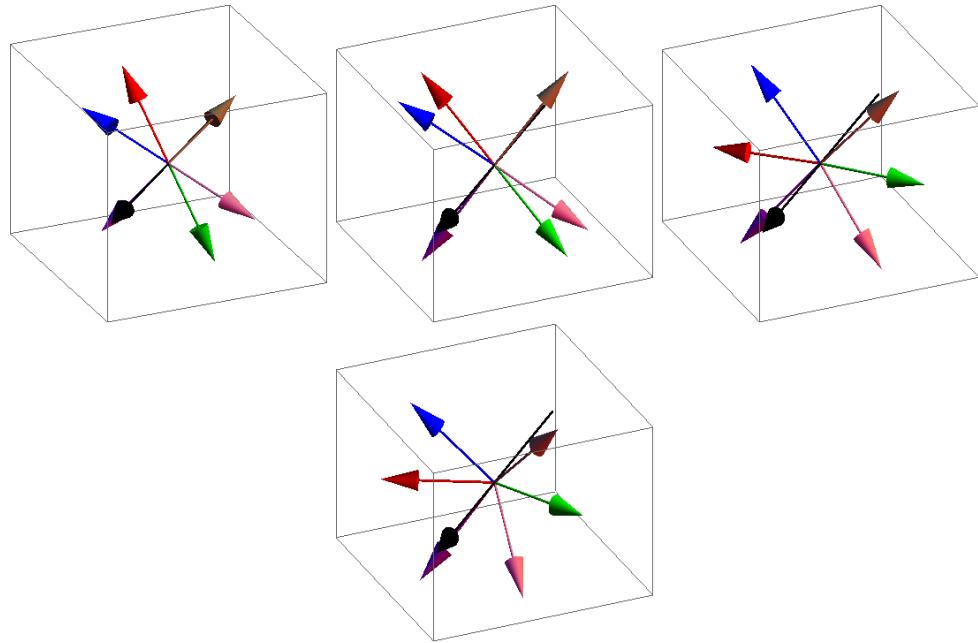


Figure 38: Snapshots of the 6 spins at  $H = 0.00, 0.0068, 0.0081$ , and  $0.05$

## 17 (110) 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.

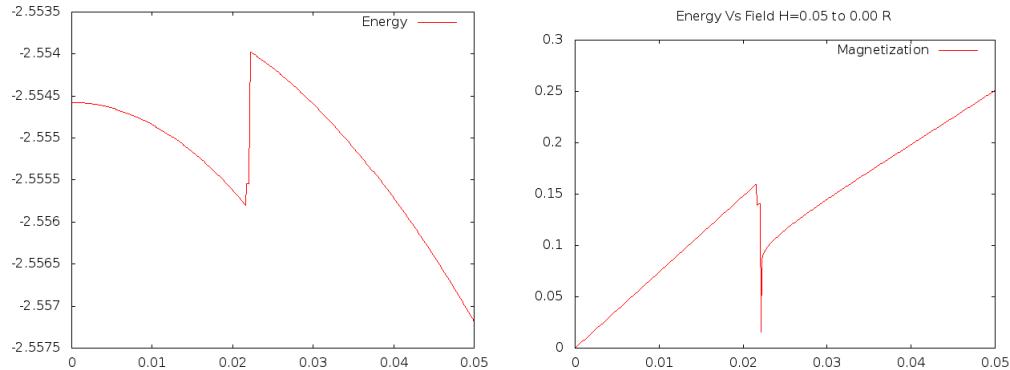


Figure 39: Energy vs decreasing field and Magnetization versus decreasing field

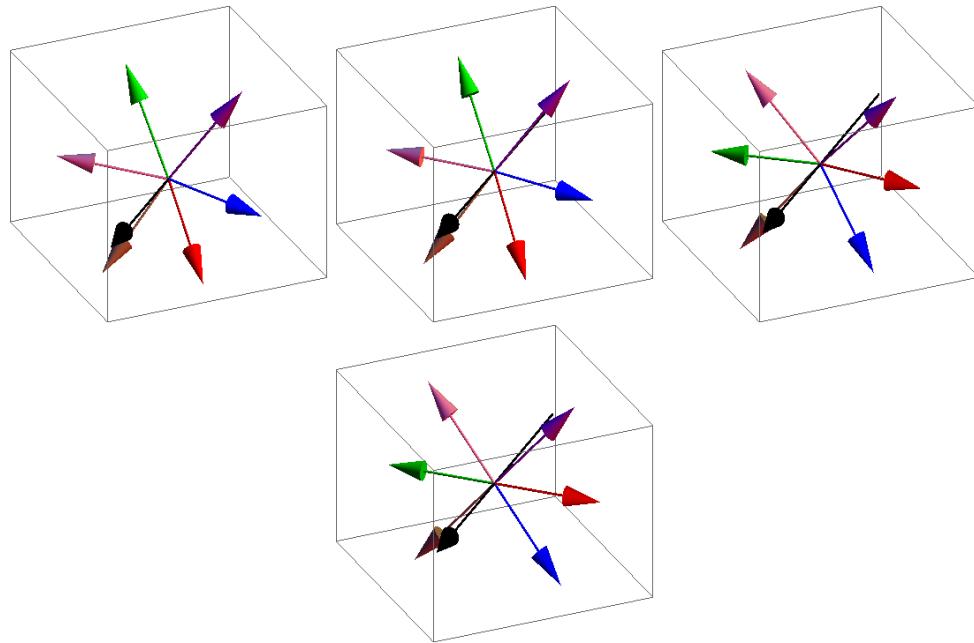


Figure 40: Snapshots at  $H=0.05$ ,  $H=0.0260$ ,  $0.0201$ , and  $0$ .

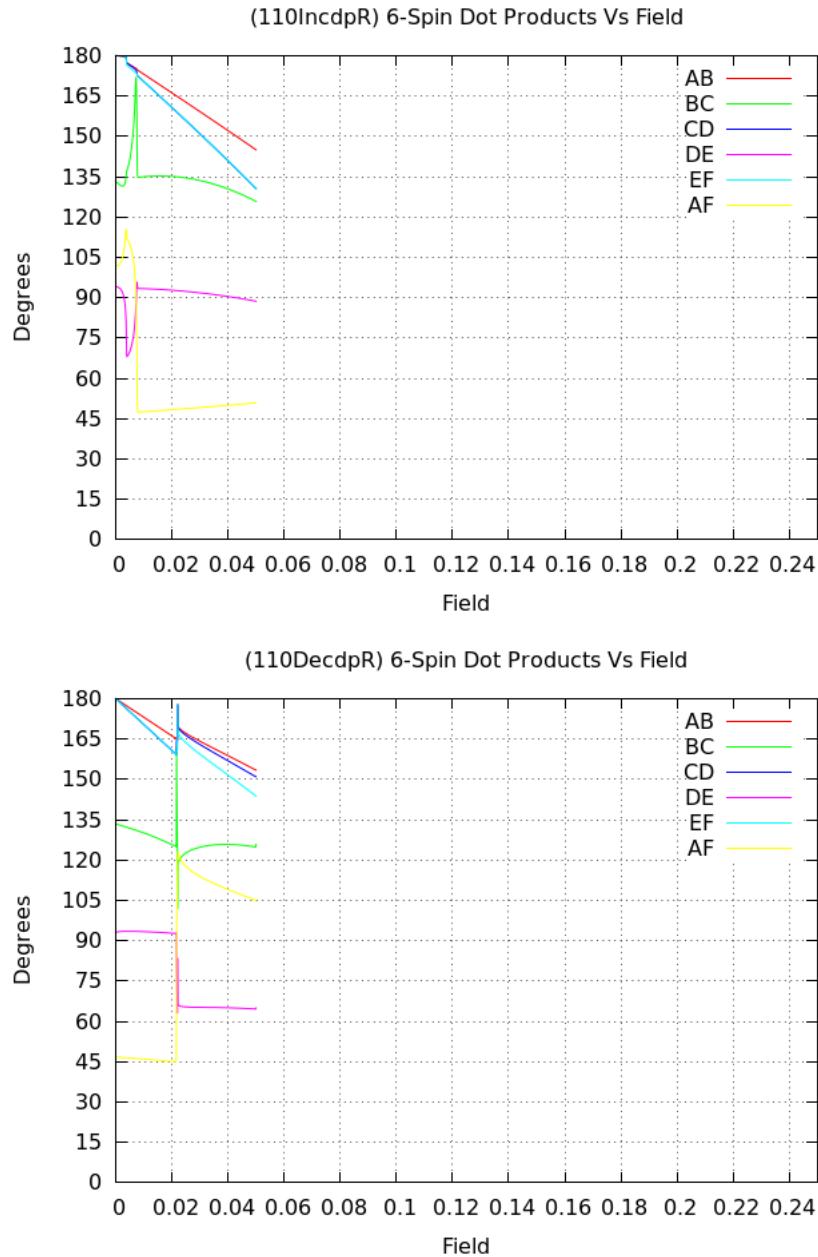


Figure 41: The curves from starting with a random initial state is different than that of starting with the ground state. The curves follow a similar trend, but are markedly different. This indicates whatever states it falls into is dependent on starting state, and that there are multiple planar states the spin configuration after transitioning. This simulation was also only run to 0.05, passed the transition point.

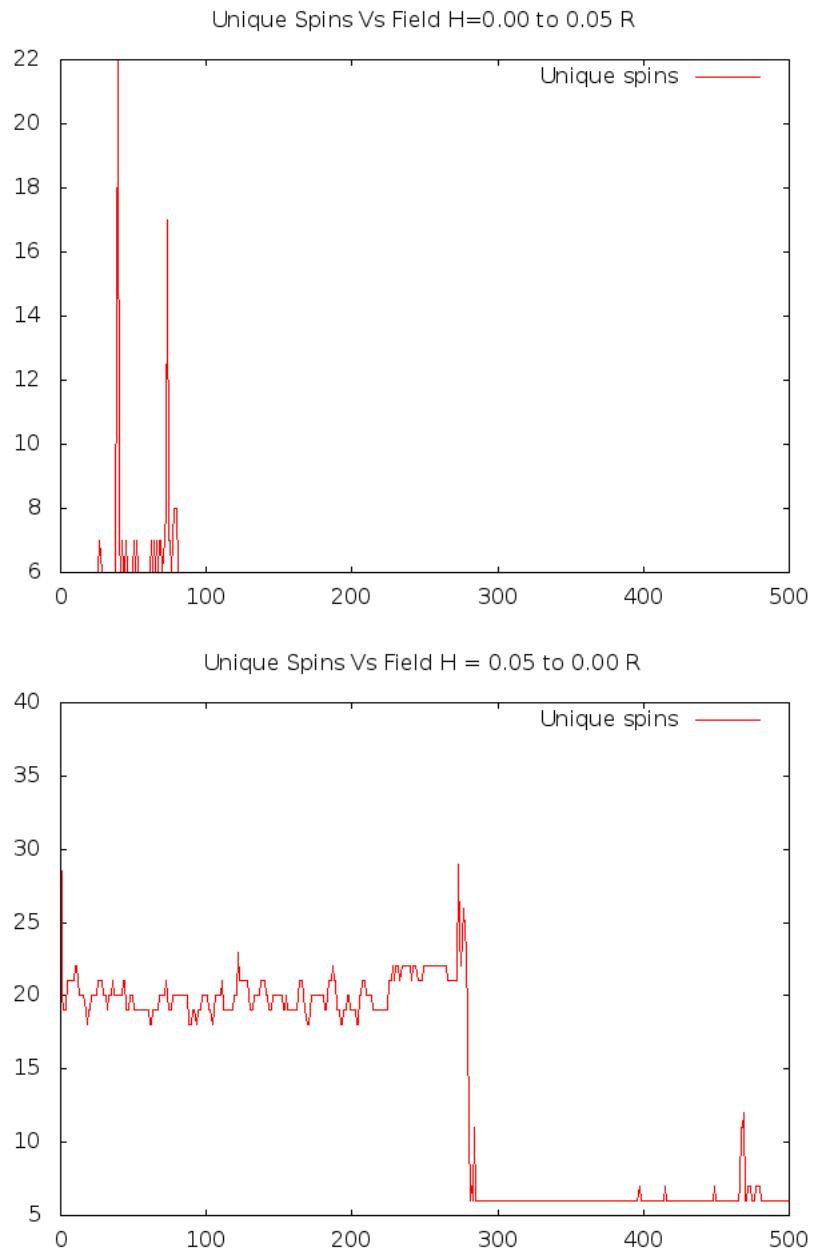


Figure 42: When decreasing the field, the lattice seems to be having trouble finding a stable 6 spin configuration. A sudden transition is observed at approximately 0.028 field, which can be observed in all graphs from this simulation.

## 18 2K (111) Increasing Field, Ground State

Steps persist in the energy graphs. This can probably be fixed by increasing precision. A sudden drop in energy occurs at field 0.006. This corresponds to the spin configuration snapping into a planar state, where the applied field vector intersects the plane. The angle of intersection is not perpendicular, but looks close to it. Once in the planar state, the spins gradually align with the field, and nothing else interesting happens.

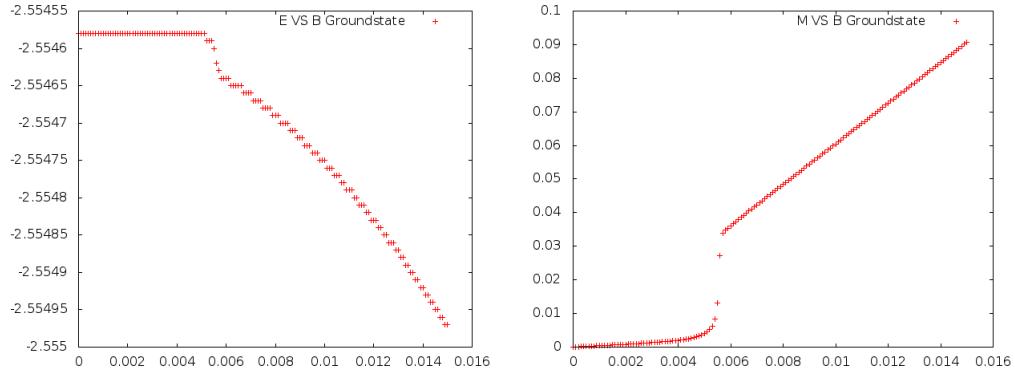


Figure 43: Energy vs increasing field and Magnetization versus increasing field

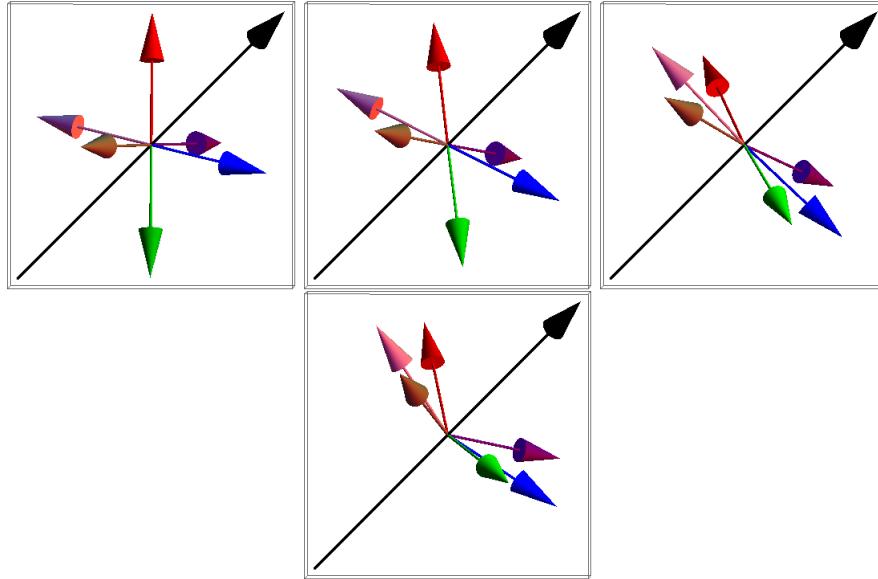


Figure 44: Snapshots of the 6 characteristic spins of the lattice at  $B=0$ ,  $B=0.0052$ ,  $B=0.0077$ , and  $B=0.05$

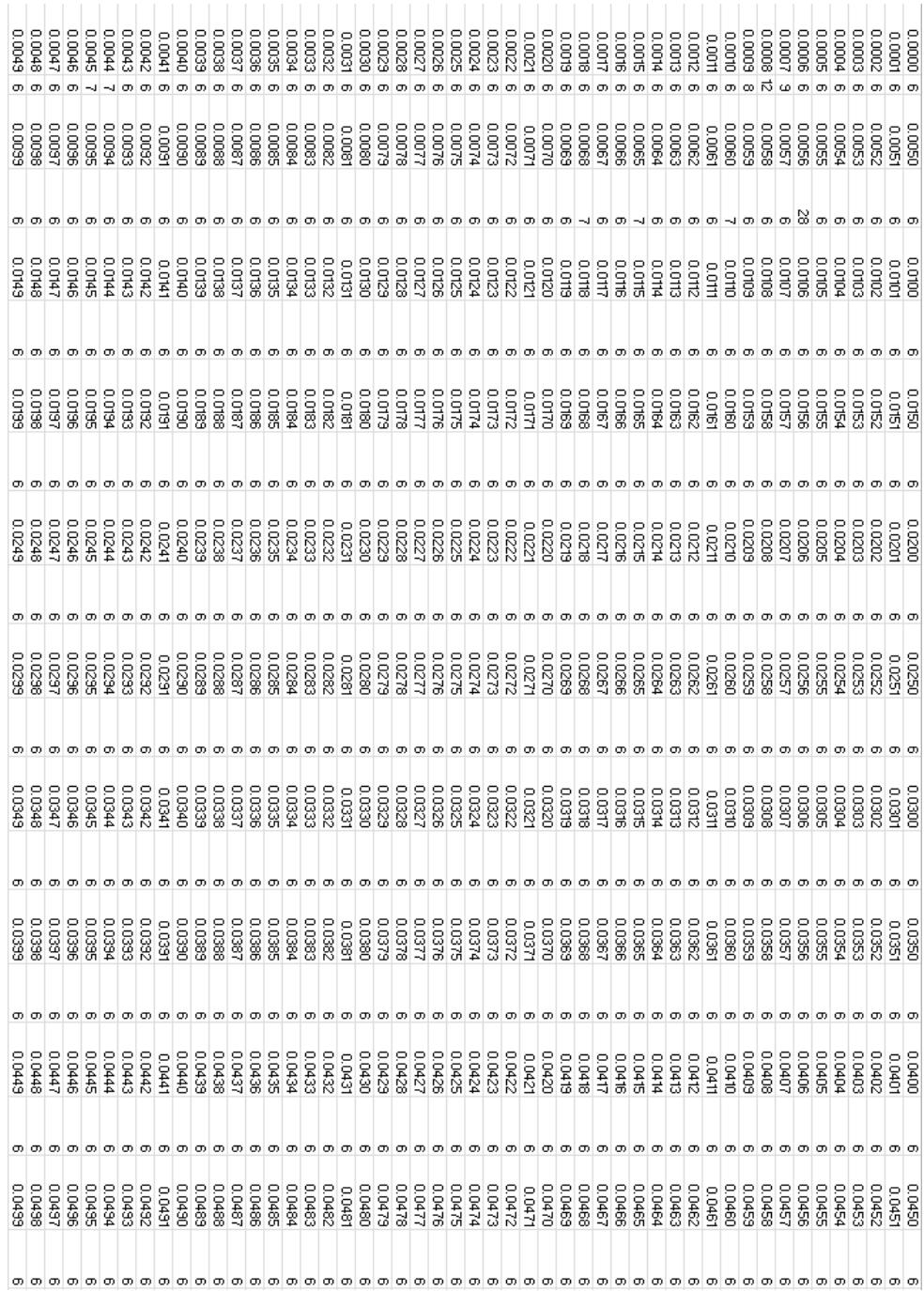


Figure 45: A chart outlining the number of unique spins within the lattice for various field magnitudes in the 111 direction. The simulation began with the groundstate configuration, and used 2000 iterations.

## 19 2K (111) Decreasing Field, Ground State

Steps persist in the energy graphs. Increasing precision can probably fix this. Unlike the case where the field was increased, a sudden transition does not occur within the spin configuration when decreasing the field. The field is initially at its highest, and the spins are partially aligned with the field. As the field is lowered, the spins gradually relax to a planar state, and do not return to the ground state that is typically observed at near zero or zero field.

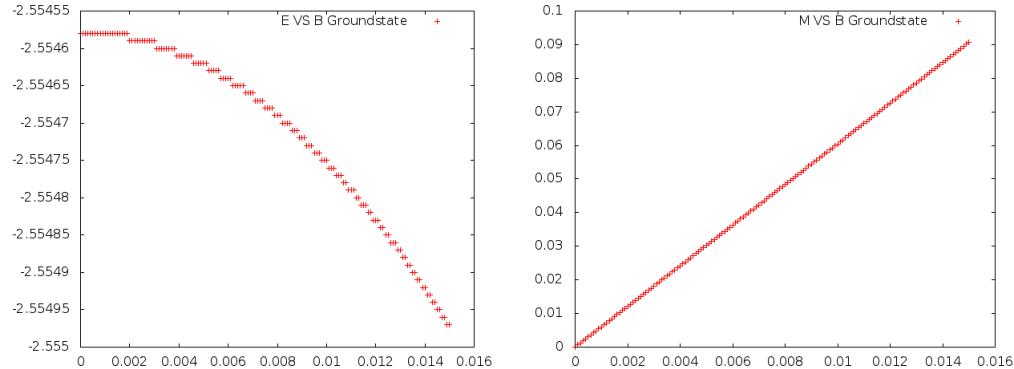


Figure 46: Energy vs decreasing field and Magnetization versus decreasing field

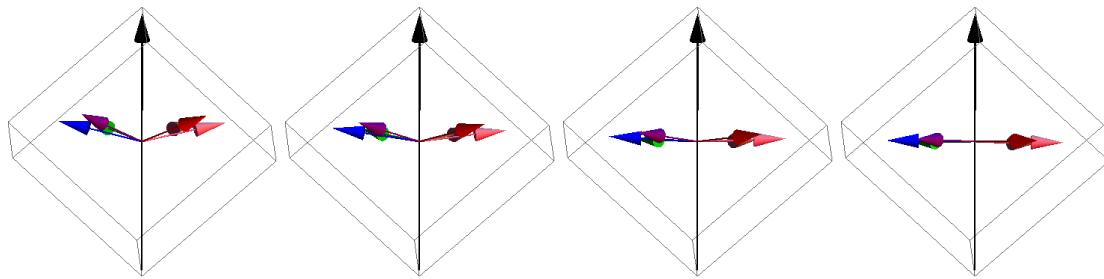


Figure 47: Snapshots of the 6 characteristic spins of the lattice at  $B=0.05$ ,  $B=0.0309$ ,  $B=0.01$ , and  $B=0.00$

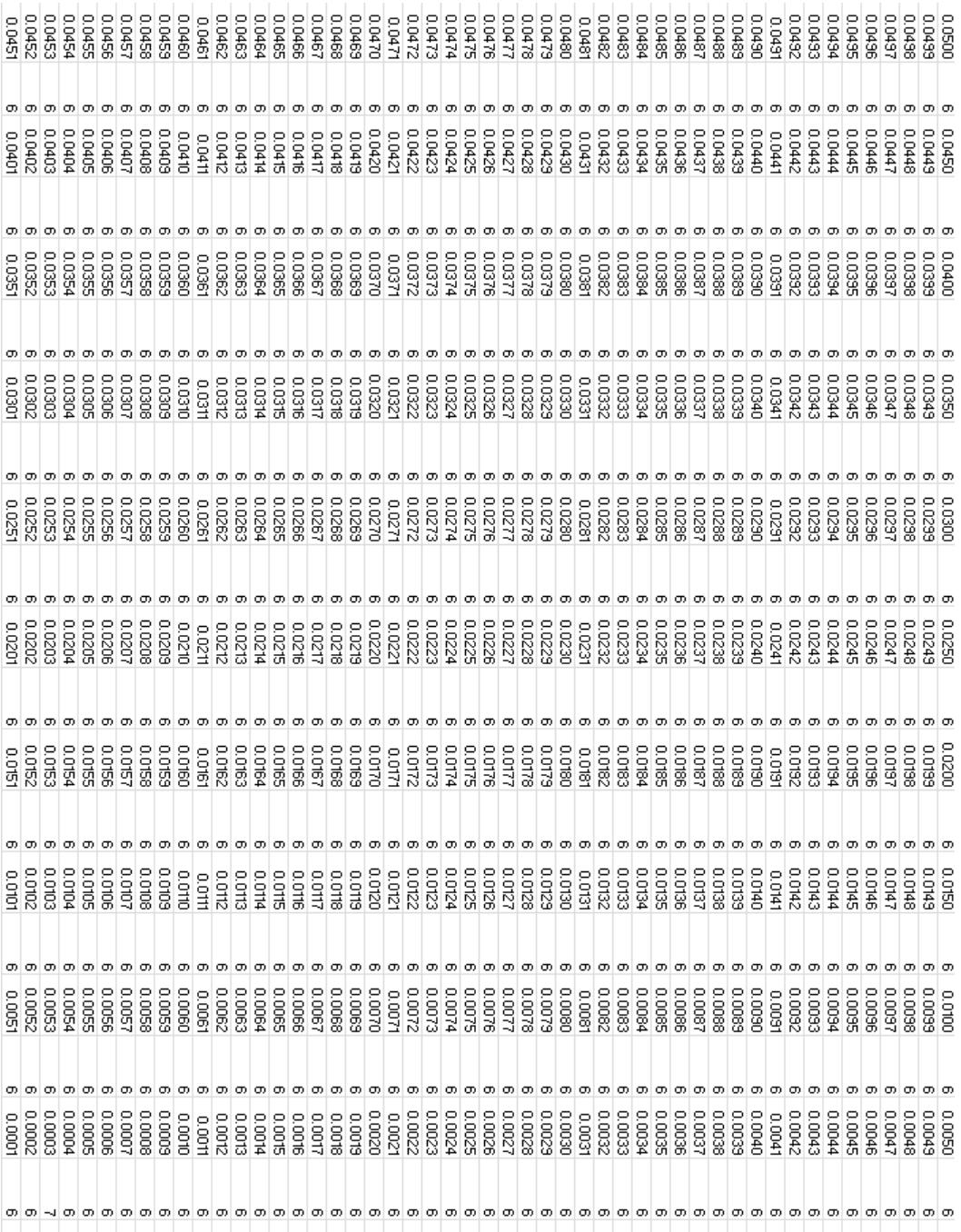


Figure 48: A chart outlining the number of unique spins within the lattice for various field magnitudes in the 111 direction for a decreasing field. The spin configuration was initially the groundstate, and used 2000 iterations.

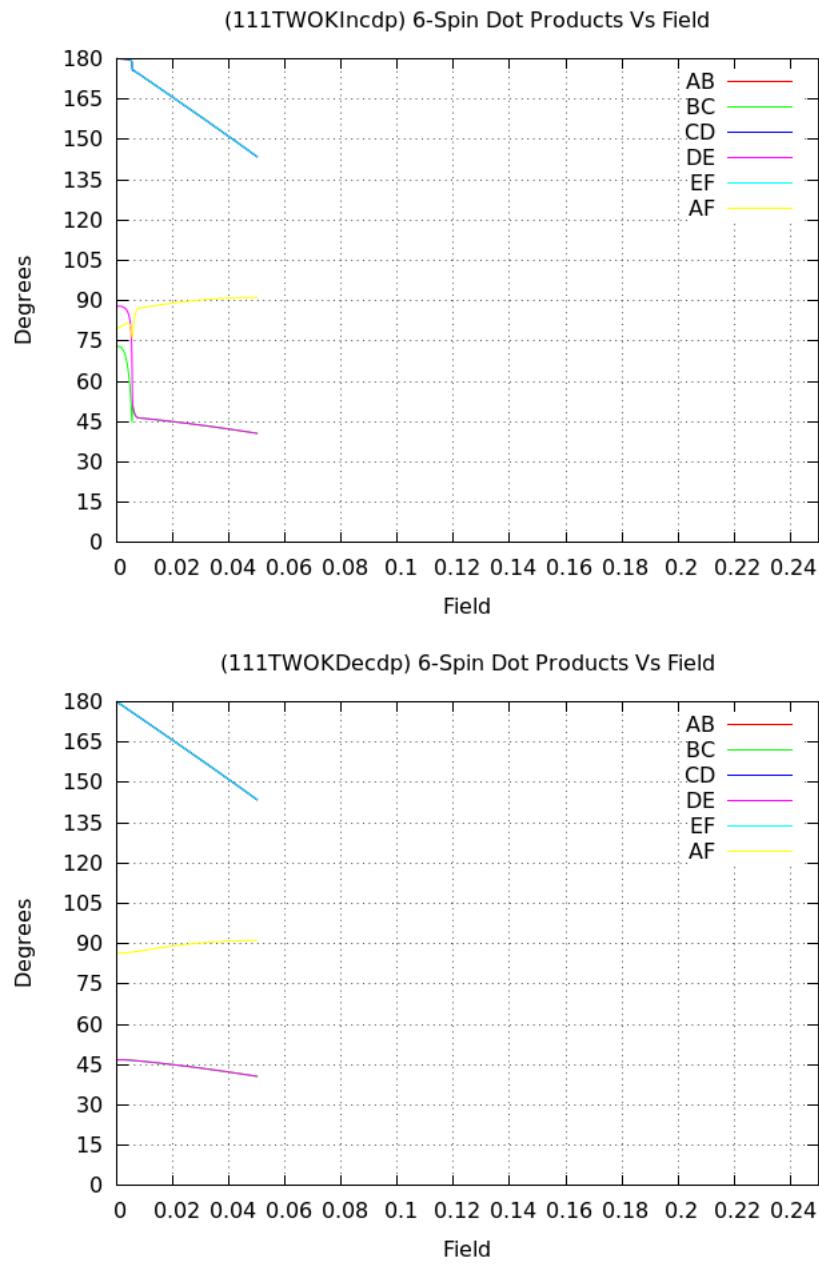


Figure 49: Dot products of the 6 characteristic spins for both increasing and decreasing fields.

## 20 2K (111) Increasing Field, Random State

Very similar to run 1, where the lattice starts off at a ground state configuration and snaps into a planar configuration, followed by gradual alignment with the field. Note: the first data point in the energy and magnetization plots were removed since it was much higher than any other points on the graph, which caused the plot to become flattened in order to fit the entire range of data onto the same plot. This is likely due to the fact that 2000 iterations is insufficient for the energy to be minimized, and so starting from a random initial configuration causes the energy of the lattice at the first field value ( $B=0$ ) to be much higher than the ground state since it has yet to become a ground state.

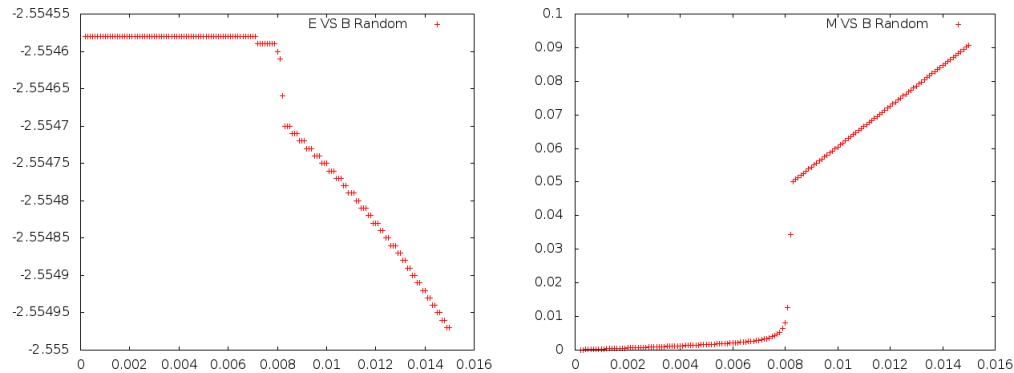


Figure 50: Energy vs increasing field and Magnetization versus increasing field

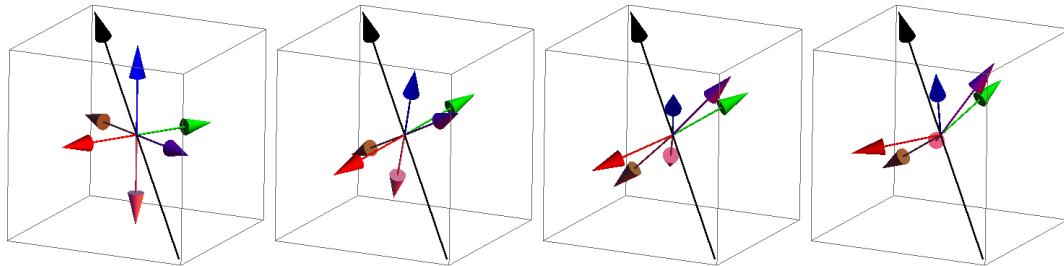


Figure 51: Snapshots of the 6 characteristic spins of the lattice. Fields not recorded, but snapshot 1 is the groundstate at zero field, the second is prior to the point of inflection, the third is immediately after the point of inflection, and the fourth is likely at 0.05, the maximum field for this simulation.

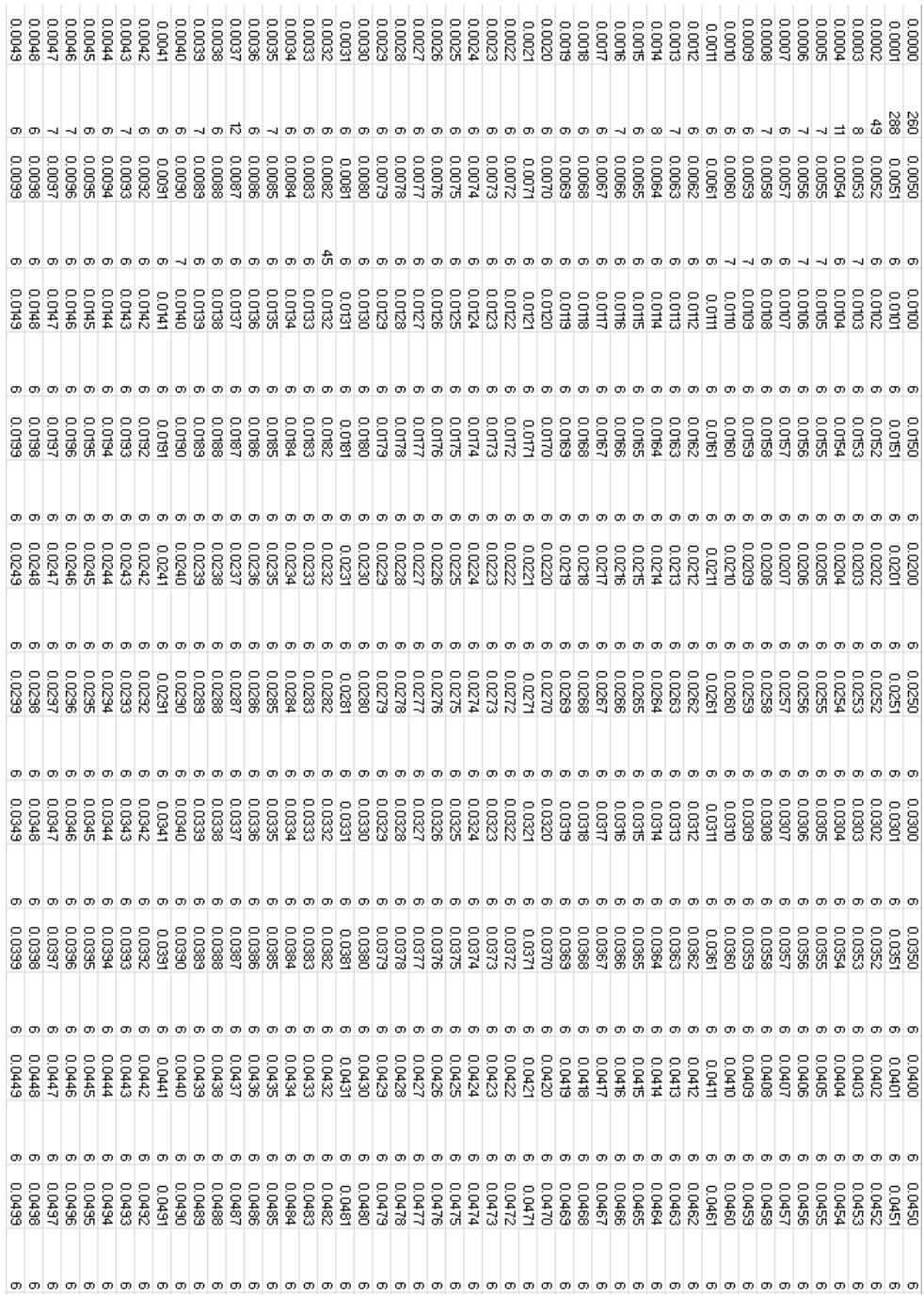


Figure 52: A chart outlining the number of unique spins within the lattice for increasing field magnitude in the 111 direction. The lattice was initially random. EFM used 2000 iterations.

## 21 2K (111) Decreasing Field, Random State

Between the first two images of the 6 spins, there is little difference even though the field had changed by about 0.03. At 0.21, the 6 spins undergo sudden and rapid changes in orientation. Eventually, the 6 spins rest in a near planar state, and gradually relax to a full planar state at  $B=0$ . When referring to the spin chart, it's clear that trying to visualize the entire lattice by choosing 6 spins won't work, since there are far more than 6 spins for the majority of fields. An alternate approach was used, which involved looking at a small, manageable section of the entire lattice.

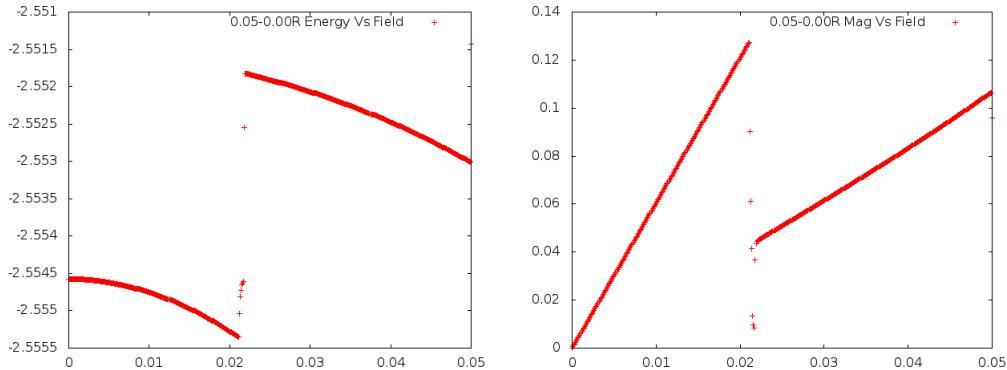


Figure 53: Energy vs decreasing field and Magnetization versus decreasing field

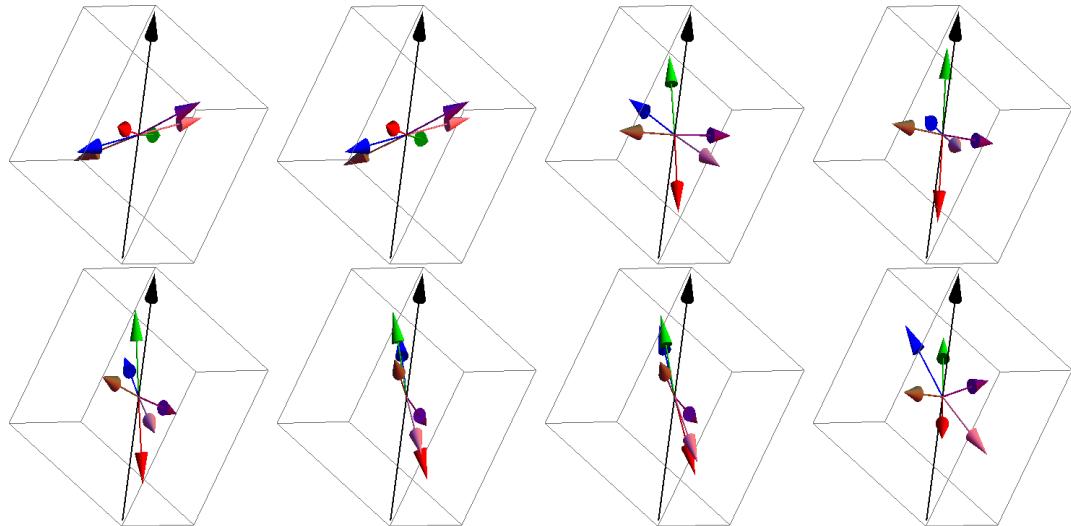


Figure 54: Snapshots of the 6 characteristic spins of the lattice over the course of increasing field

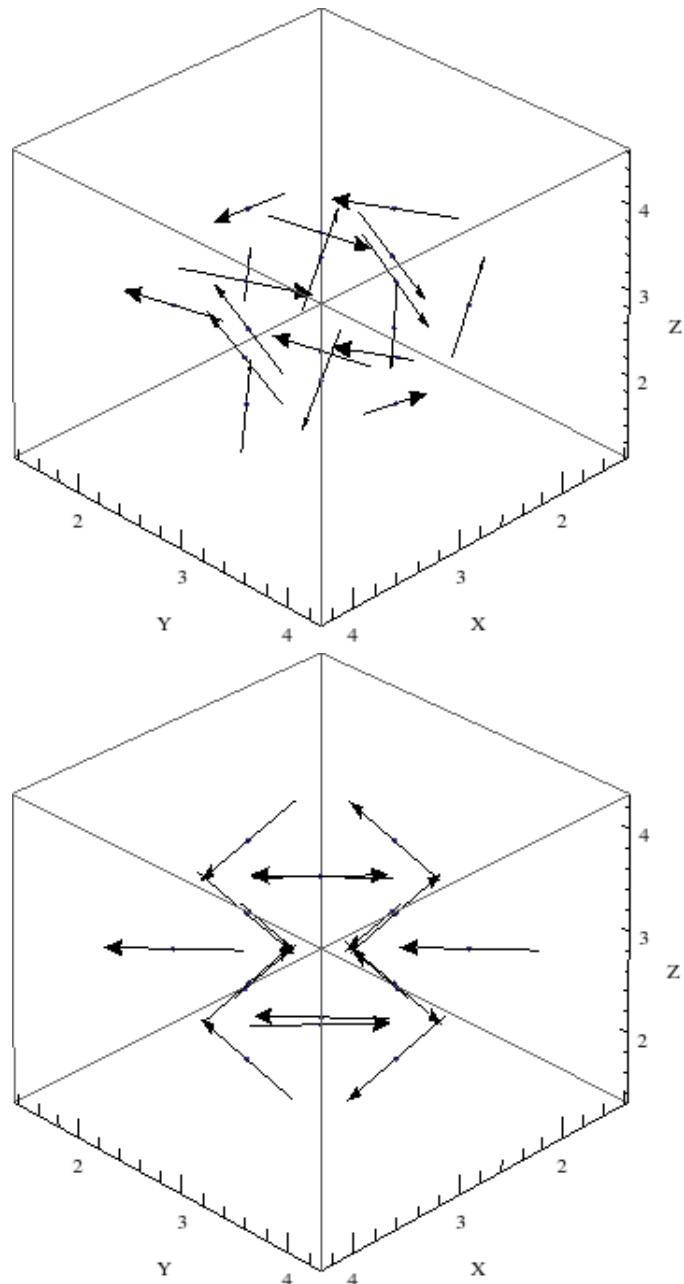


Figure 55: Visualization of a small section of the entire lattice used in the 2K iteration 111 decreasing field simulation. The spins are initially highly disordered, until they snap into a final planar configuration. The field at which this transition occurred can be deduced from the spin chart for this simulation. Ie, at  $H=0.02$  when the number of unique spins equal 6.

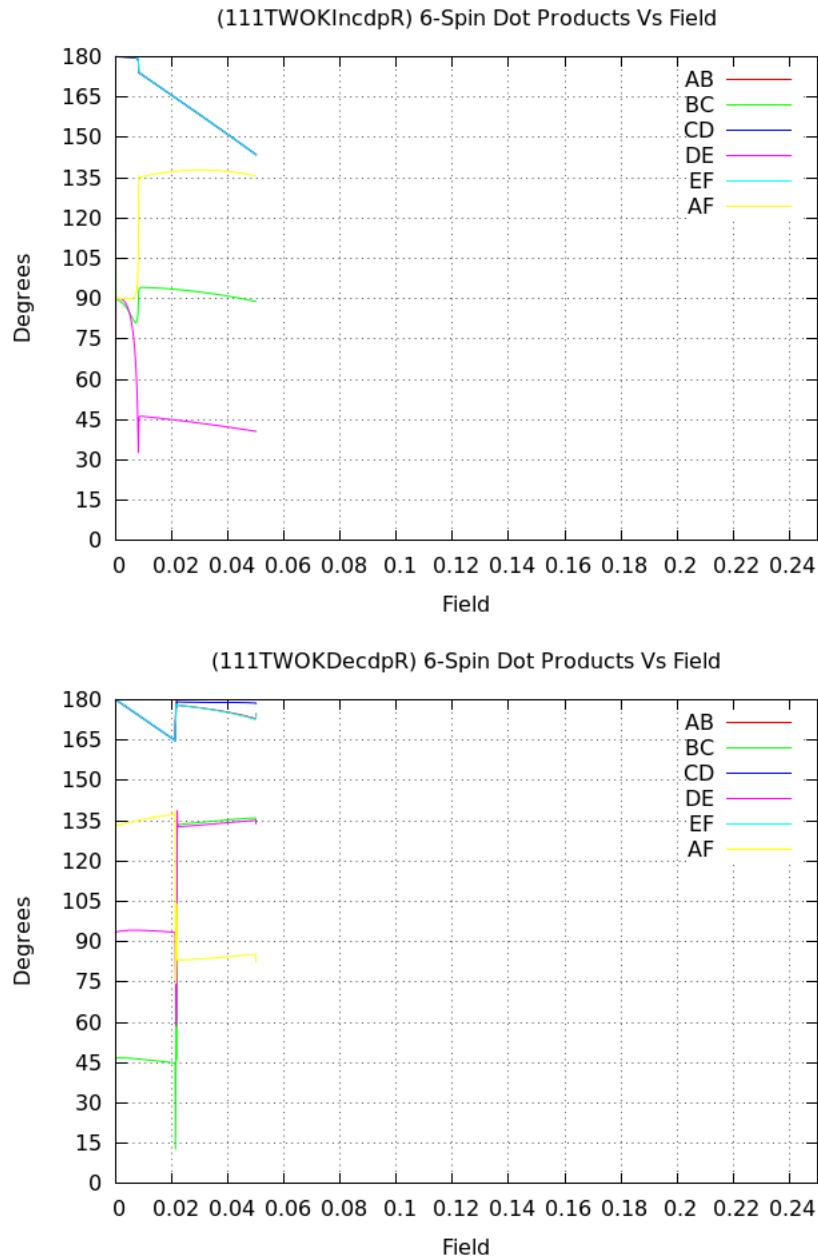


Figure 56: Dot products of the characteristic spins for increasing and decreasing field. Since this was a preliminary simulation, the field was only increased to 0.05.

0.0500	102	0.045	84	0.04	84	0.035	88	0.03	83	0.025	78	0.02	6	0.015	6	0.005
0.0499	92	0.0449	86	0.039	82	0.0349	89	0.0289	82	0.0249	78	0.019	6	0.049	6	0.009
0.0498	86	0.0448	86	0.0398	88	0.0348	88	0.0298	82	0.0248	78	0.019	6	0.0098	6	0.0048
0.0497	86	0.0447	82	0.0397	88	0.0347	88	0.0287	82	0.0247	78	0.019	6	0.047	6	0.0047
0.0496	86	0.0446	82	0.0396	90	0.0346	88	0.0296	82	0.0246	78	0.019	6	0.046	6	0.0046
0.0495	90	0.0445	84	0.0395	88	0.0345	88	0.0295	80	0.0245	80	0.0195	6	0.045	6	0.0045
0.0494	86	0.0444	89	0.0394	90	0.0344	88	0.0294	80	0.0244	80	0.0194	6	0.044	6	0.0044
0.0493	88	0.0443	84	0.0393	90	0.0343	86	0.0293	80	0.0243	80	0.0193	6	0.043	6	0.0043
0.0492	86	0.0442	82	0.0392	84	0.0342	83	0.0292	82	0.0242	78	0.0192	6	0.042	6	0.0042
0.0491	88	0.0441	82	0.0391	86	0.0341	82	0.0291	80	0.0241	78	0.0191	6	0.041	6	0.0041
0.0490	88	0.044	85	0.039	86	0.034	84	0.029	80	0.024	78	0.019	6	0.04	6	0.004
0.0489	86	0.0439	84	0.0389	89	0.0339	84	0.0289	81	0.0189	6	0.039	6	0.0039	6	0.0039
0.0488	86	0.0438	82	0.0388	88	0.0338	84	0.0288	80	0.0238	81	0.0188	6	0.038	6	0.0038
0.0487	86	0.0437	82	0.0387	88	0.0337	84	0.0287	78	0.0237	80	0.0187	6	0.037	6	0.0037
0.0486	84	0.0436	82	0.0386	88	0.0336	84	0.0286	79	0.0236	82	0.0186	6	0.036	6	0.0036
0.0485	84	0.0435	82	0.0385	88	0.0335	84	0.0285	78	0.0235	80	0.0185	6	0.035	6	0.0035
0.0484	84	0.0434	82	0.0384	89	0.0334	86	0.0284	76	0.0234	82	0.0184	6	0.034	6	0.0034
0.0483	84	0.0433	84	0.0383	89	0.0333	88	0.0283	78	0.0233	83	0.0183	6	0.033	6	0.0033
0.0482	84	0.0432	82	0.0382	86	0.0332	88	0.0282	76	0.0232	83	0.0182	6	0.032	6	0.0032
0.0481	82	0.0431	82	0.0381	86	0.0331	88	0.0281	80	0.0231	84	0.0181	6	0.031	6	0.0031
0.0480	82	0.043	82	0.038	88	0.033	88	0.028	80	0.023	84	0.018	6	0.03	6	0.003
0.0479	82	0.0429	82	0.0379	88	0.0329	88	0.0279	80	0.0229	82	0.0184	6	0.034	6	0.0034
0.0478	84	0.0428	80	0.0378	95	0.0328	88	0.0278	76	0.0228	84	0.0178	6	0.028	6	0.0028
0.0477	84	0.0427	82	0.0377	95	0.0327	88	0.0277	78	0.0227	83	0.0177	6	0.027	6	0.0027
0.0476	86	0.0426	82	0.0376	96	0.0326	88	0.0276	82	0.0226	83	0.0176	6	0.026	6	0.0026
0.0475	86	0.0425	84	0.0375	96	0.0325	90	0.0275	82	0.0225	83	0.0175	6	0.025	6	0.0025
0.0474	86	0.0424	80	0.0374	98	0.0324	88	0.0274	82	0.0224	84	0.0174	6	0.024	6	0.0024
0.0473	86	0.0423	80	0.0373	98	0.0323	88	0.0273	83	0.0223	86	0.0173	6	0.023	6	0.0023
0.0472	90	0.0422	80	0.0372	96	0.0322	88	0.0272	84	0.0222	87	0.0172	6	0.022	6	0.0022
0.0471	86	0.0421	86	0.0371	96	0.0321	90	0.0271	91	0.0221	85	0.0171	6	0.021	6	0.0021
0.0470	82	0.042	88	0.037	94	0.032	90	0.027	91	0.022	93	0.017	6	0.0207	6	0.00207
0.0469	82	0.0419	88	0.0369	92	0.0319	90	0.0269	90	0.0218	110	0.0169	6	0.019	6	0.0019
0.0468	84	0.0418	88	0.0366	92	0.0318	88	0.0268	90	0.0218	50	0.0168	6	0.018	6	0.0018
0.0467	84	0.0417	88	0.0367	94	0.0317	88	0.0267	88	0.0217	29	0.0167	6	0.017	6	0.0017
0.0466	86	0.0416	88	0.0366	92	0.0316	86	0.0266	88	0.0216	3	0.0166	6	0.016	6	0.0016
0.0465	86	0.0415	86	0.0365	92	0.0315	86	0.0265	86	0.0215	11	0.0165	6	0.015	6	0.0015
0.0464	86	0.0414	88	0.0364	90	0.0314	86	0.0264	84	0.0214	3	0.0164	6	0.014	6	0.0014
0.0463	84	0.0413	84	0.0363	86	0.0313	86	0.0263	86	0.0213	9	0.0163	6	0.013	6	0.0013
0.0462	84	0.0412	82	0.0362	86	0.0312	86	0.0262	85	0.022	10	0.0162	6	0.012	6	0.0012
0.0461	84	0.0411	82	0.0361	90	0.0311	86	0.0261	82	0.0211	8	0.0161	6	0.011	6	0.0011
0.0460	82	0.041	82	0.036	90	0.031	86	0.026	82	0.021	6	0.016	6	0.006	6	0.0006
0.0459	82	0.0409	84	0.0359	90	0.0309	86	0.0259	82	0.0209	6	0.0159	6	0.0059	6	0.0009
0.0458	84	0.0408	86	0.0358	90	0.0308	84	0.0258	82	0.0208	6	0.0158	6	0.0058	6	0.0008
0.0457	84	0.0407	86	0.0357	89	0.0307	84	0.0257	80	0.0207	6	0.0157	6	0.0057	6	0.0007
0.0456	86	0.0406	84	0.0356	90	0.0306	82	0.0256	80	0.0206	6	0.0156	6	0.0056	6	0.0006
0.0455	86	0.0405	84	0.0355	90	0.0305	84	0.0255	80	0.0205	6	0.0155	6	0.0055	6	0.0005
0.0454	86	0.0404	84	0.0354	90	0.0304	84	0.0254	82	0.0204	6	0.0154	6	0.0054	6	0.0004
0.0453	86	0.0403	84	0.0353	90	0.0303	82	0.0253	82	0.0203	6	0.0153	6	0.0053	6	0.0003
0.0452	86	0.0402	82	0.0352	82	0.0252	82	0.0202	6	0.0152	6	0.0052	6	0.0002	6	0.0002
0.0451	84	0.0401	90	0.0301	82	0.0251	78	0.0201	6	0.0151	6	0.0051	6	0.0001	6	0.0001

Figure 57: The number of unique spins within the lattice for this simulation was extremely high. This is likely a result of insufficient EFM iterations

## 22 3K (111) Increasing Field, Ground State

Steps persist in the energy graphs when plotting on a smaller scale. This can probably be fixed by increasing precision. A sudden drop in energy occurs at field 0.0049. There is little difference between the 2000 and 3000 step simulations for increasing field up to  $H=0.05$ . The 2000 and 3000 iterations can't be compared for fields beyond that, since the 2000 step simulation was only run to  $H=0.05$ .

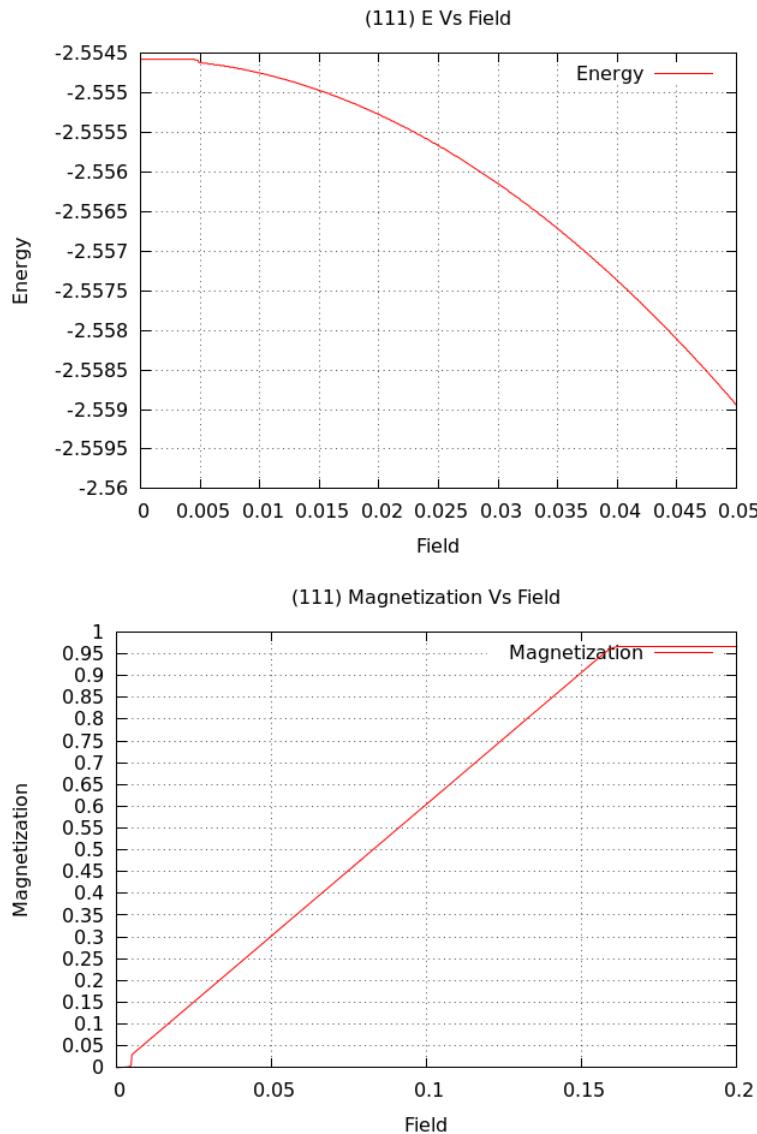


Figure 58: Energy vs increasing field and Magnetization versus increasing field

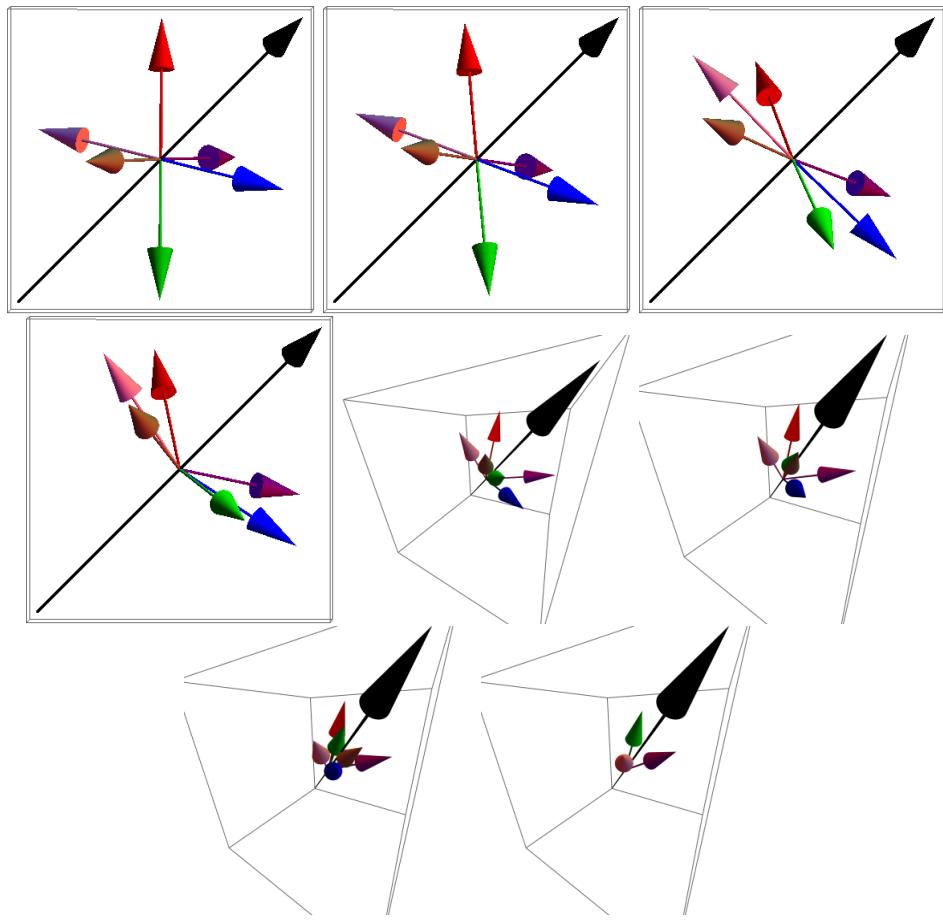


Figure 59: Snapshots of the 6 characteristic spins of the lattice at  $H=0, 0.0040, 0.0055, 0.05, 0.140, 0.152, 0.158, 0.172$ . As the spins close up, the brown and green spins become parallel, then unalign. Finally, the 6 spin system appears to reduce to a 3-spin system at  $H=0.17$ .

0.0000	6	0.005	6	0.01	6	0.015	6	0.02	6	0.025	6	0.03	6	0.035	6	0.04	6	0.045	6
0.0001	6	0.0051	6	0.0101	6	0.0151	6	0.0201	6	0.0251	6	0.0301	6	0.0351	6	0.0401	6	0.0451	6
0.0002	6	0.0052	7	0.0102	6	0.0152	6	0.0202	6	0.0252	6	0.0302	6	0.0352	6	0.0402	6	0.0452	6
0.0003	6	0.0053	6	0.0103	6	0.0153	6	0.0203	6	0.0253	6	0.0303	6	0.0353	6	0.0403	6	0.0453	6
0.0004	6	0.0054	6	0.0104	6	0.0154	6	0.0204	6	0.0254	6	0.0304	6	0.0354	6	0.0404	6	0.0454	6
0.0005	13	0.0055	6	0.0105	6	0.0155	6	0.0205	6	0.0255	6	0.0305	6	0.0355	6	0.0405	6	0.0455	6
0.0006	7	0.0056	6	0.0106	6	0.0156	6	0.0206	6	0.0256	6	0.0306	6	0.0356	6	0.0406	6	0.0456	6
0.0007	6	0.0057	6	0.0107	6	0.0157	6	0.0207	6	0.0257	6	0.0307	6	0.0357	6	0.0407	6	0.0457	6
0.0008	6	0.0058	6	0.0108	6	0.0158	6	0.0208	6	0.0258	6	0.0308	6	0.0358	6	0.0408	6	0.0458	6
0.0009	6	0.0059	6	0.0109	6	0.0159	6	0.0209	6	0.0259	6	0.0309	6	0.0359	6	0.0409	6	0.0459	6
0.0010	7	0.006	6	0.011	6	0.016	6	0.021	6	0.026	6	0.031	6	0.036	6	0.041	6	0.046	6
0.0011	6	0.0061	6	0.0111	6	0.0161	6	0.0211	6	0.0261	6	0.0311	6	0.0361	6	0.0411	6	0.0461	6
0.0012	6	0.0062	6	0.0112	6	0.0162	6	0.0212	6	0.0262	6	0.0312	6	0.0362	6	0.0412	6	0.0462	6
0.0013	6	0.0063	6	0.0113	6	0.0163	6	0.0213	6	0.0263	6	0.0313	6	0.0363	6	0.0413	6	0.0463	6
0.0014	6	0.0064	6	0.0114	6	0.0164	6	0.0214	6	0.0264	6	0.0314	6	0.0364	6	0.0414	6	0.0464	6
0.0015	6	0.0065	6	0.0115	6	0.0165	6	0.0215	6	0.0265	6	0.0315	6	0.0365	6	0.0415	6	0.0465	6
0.0016	6	0.0066	6	0.0116	6	0.0166	6	0.0216	6	0.0266	6	0.0316	6	0.0366	6	0.0416	6	0.0466	6
0.0017	6	0.0067	6	0.0117	6	0.0167	6	0.0217	6	0.0267	6	0.0317	6	0.0367	6	0.0417	6	0.0467	6
0.0018	6	0.0068	6	0.0118	6	0.0168	6	0.0218	6	0.0268	6	0.0318	6	0.0368	6	0.0418	6	0.0468	6
0.0019	7	0.0069	6	0.0119	6	0.0169	6	0.0219	6	0.0269	6	0.0319	6	0.0369	6	0.0419	6	0.0469	6
0.0020	6	0.007	6	0.012	6	0.017	6	0.022	6	0.027	6	0.032	6	0.037	6	0.042	6	0.047	6
0.0021	6	0.0071	6	0.0121	6	0.0171	6	0.0221	6	0.0271	6	0.0321	6	0.0371	6	0.0421	6	0.0471	6
0.0022	6	0.0072	6	0.0122	6	0.0172	6	0.0222	6	0.0272	6	0.0322	6	0.0372	6	0.0422	6	0.0472	6
0.0023	6	0.0073	6	0.0123	6	0.0173	6	0.0223	6	0.0273	6	0.0323	6	0.0373	6	0.0423	6	0.0473	6
0.0024	6	0.0074	6	0.0124	6	0.0174	6	0.0224	6	0.0274	6	0.0324	6	0.0374	6	0.0424	6	0.0474	6
0.0025	6	0.0075	6	0.0125	6	0.0175	6	0.0225	6	0.0275	6	0.0325	6	0.0375	6	0.0425	6	0.0475	6
0.0026	6	0.0076	6	0.0126	6	0.0176	6	0.0226	6	0.0276	6	0.0326	6	0.0376	6	0.0426	6	0.0476	6
0.0027	6	0.0077	6	0.0127	6	0.0177	6	0.0227	6	0.0277	6	0.0327	6	0.0377	6	0.0427	6	0.0477	6
0.0028	6	0.0078	6	0.0128	6	0.0178	6	0.0228	6	0.0278	6	0.0328	6	0.0378	6	0.0428	6	0.0478	6
0.0029	6	0.0079	6	0.0129	6	0.0179	6	0.0229	6	0.0279	6	0.0329	6	0.0379	6	0.0429	6	0.0479	6
0.0030	6	0.008	6	0.013	6	0.018	6	0.023	6	0.028	6	0.033	6	0.038	6	0.043	6	0.048	6
0.0031	6	0.0081	6	0.0131	6	0.0181	6	0.0231	6	0.0281	6	0.0331	6	0.0381	6	0.0431	6	0.0481	6
0.0032	6	0.0082	6	0.0132	6	0.0182	6	0.0232	6	0.0282	6	0.0332	6	0.0382	6	0.0432	6	0.0482	6
0.0033	6	0.0083	6	0.0133	6	0.0183	6	0.0233	6	0.0283	6	0.0333	6	0.0383	6	0.0433	6	0.0483	6
0.0034	6	0.0084	6	0.0134	6	0.0184	6	0.0234	6	0.0284	6	0.0334	6	0.0384	6	0.0434	6	0.0484	6
0.0035	6	0.0085	6	0.0135	6	0.0185	6	0.0235	6	0.0285	6	0.0335	6	0.0385	6	0.0435	6	0.0485	6
0.0036	6	0.0086	6	0.0136	6	0.0186	6	0.0236	6	0.0286	6	0.0336	6	0.0386	6	0.0436	6	0.0486	6
0.0037	6	0.0087	6	0.0137	6	0.0187	6	0.0237	6	0.0287	6	0.0337	6	0.0387	6	0.0437	6	0.0487	6
0.0038	6	0.0088	6	0.0138	6	0.0188	6	0.0238	6	0.0288	6	0.0338	6	0.0388	6	0.0438	6	0.0488	6
0.0039	6	0.0089	6	0.0139	6	0.0189	6	0.0239	6	0.0289	6	0.0339	6	0.0389	6	0.0439	6	0.0489	6
0.0040	6	0.009	6	0.014	6	0.019	6	0.024	6	0.029	6	0.034	6	0.039	6	0.044	6	0.049	6
0.0041	6	0.0091	6	0.0141	6	0.0191	6	0.0241	6	0.0291	6	0.0341	6	0.0391	6	0.0441	6	0.0491	6
0.0042	6	0.0092	6	0.0142	6	0.0192	6	0.0242	6	0.0292	6	0.0342	6	0.0392	6	0.0442	6	0.0492	6
0.0043	6	0.0093	6	0.0143	6	0.0193	6	0.0243	6	0.0293	6	0.0343	6	0.0393	6	0.0443	6	0.0493	6
0.0044	6	0.0094	6	0.0144	6	0.0194	6	0.0244	6	0.0294	6	0.0344	6	0.0394	6	0.0444	6	0.0494	6
0.0045	6	0.0095	6	0.0145	6	0.0195	6	0.0245	6	0.0295	6	0.0345	6	0.0395	6	0.0445	6	0.0495	6
0.0046	6	0.0096	6	0.0146	6	0.0196	6	0.0246	6	0.0296	6	0.0346	6	0.0396	6	0.0446	6	0.0496	6
0.0047	6	0.0097	6	0.0147	6	0.0197	6	0.0247	6	0.0297	6	0.0347	6	0.0397	6	0.0447	6	0.0497	6
0.0048	6	0.0098	6	0.0148	6	0.0198	6	0.0248	6	0.0298	6	0.0348	6	0.0398	6	0.0448	6	0.0498	6
0.0049	9	0.0099	6	0.0149	6	0.0199	6	0.0249	6	0.0299	6	0.0349	6	0.0399	6	0.0449	6	0.0499	6

Figure 60: A noticeable change in the number of unique spins occurs at 0.0049, coinciding with the transition in the energy and magnetization graphs. This chart does not include data on the lattice at fields beyond 0.05.

## 23 3K (111) Decreasing Field, Ground State

No transition is observed at low field in this scenario, similar to the 2000 step case. A transition does occur at high field when the lattice is released from a saturated state. Once released from the saturated state, the system expands from the saturated 3-spin system into the typically observed 6-spin system. Finally, the spin configuration becomes planar at zero field. The 111 field direction is the only direction that creates a 3-spin system out of all directions tested. The final configuration is characterized by theta=52.1404 degrees and phi=-116.39 degrees.

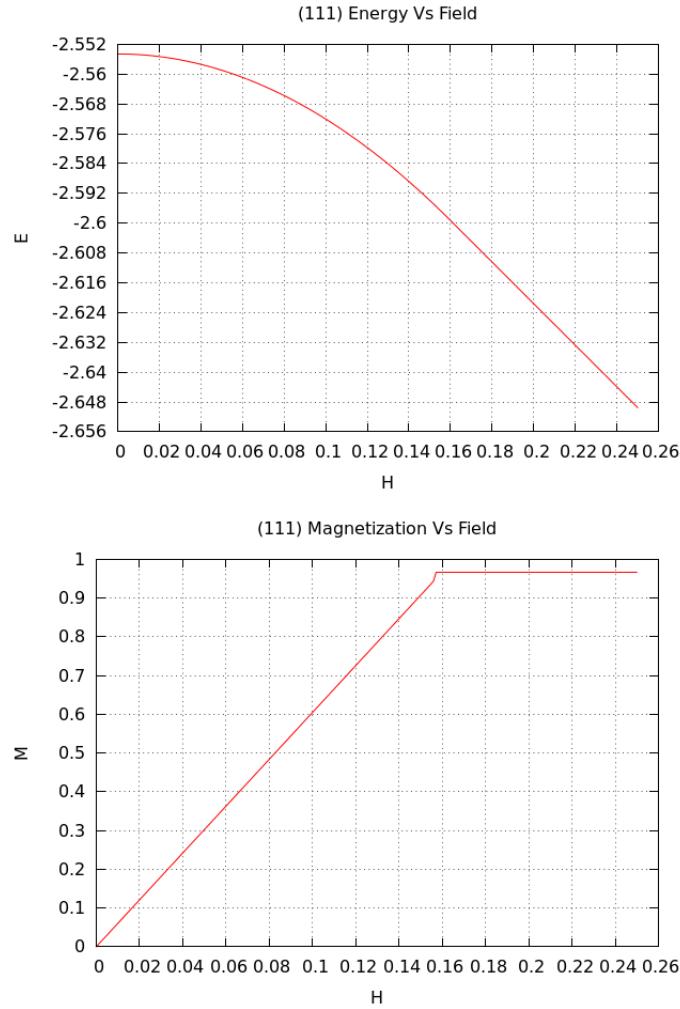


Figure 61: Energy vs decreasing field and Magnetization versus decreasing field

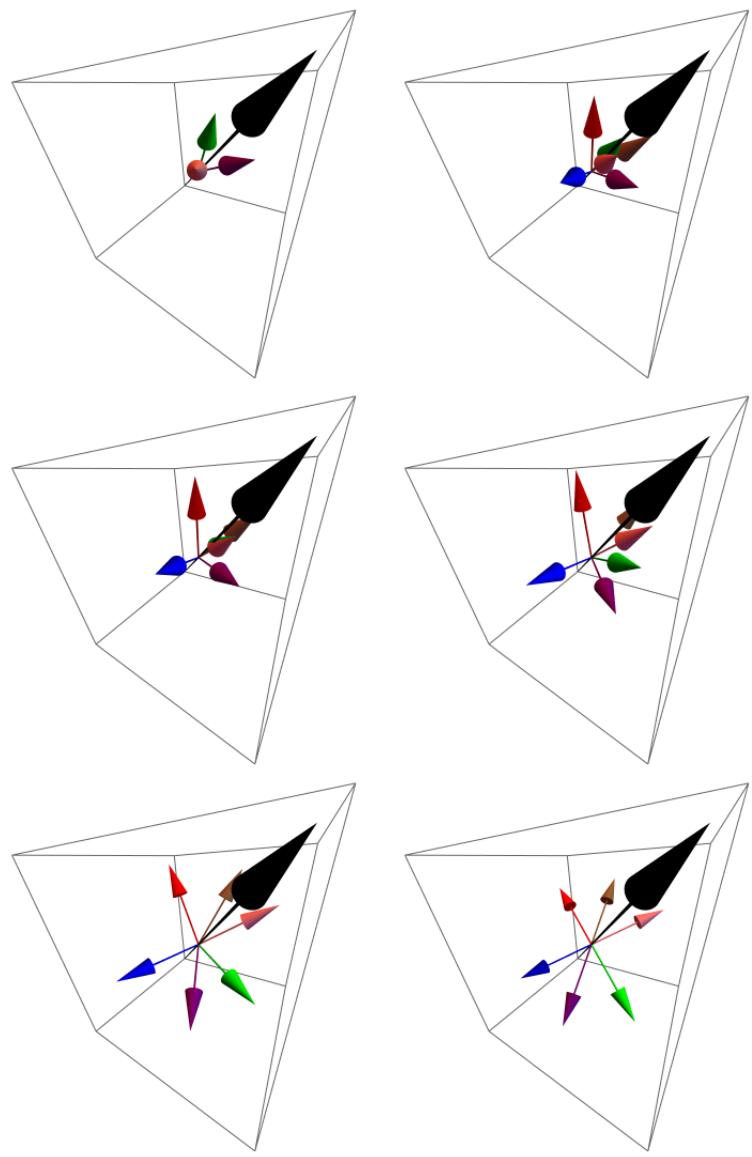


Figure 62: Snapshots of the 6 characteristic spins of the lattice at  $H=0.25, 0.156, 0.152, 0.136, 0.081$ , and 0

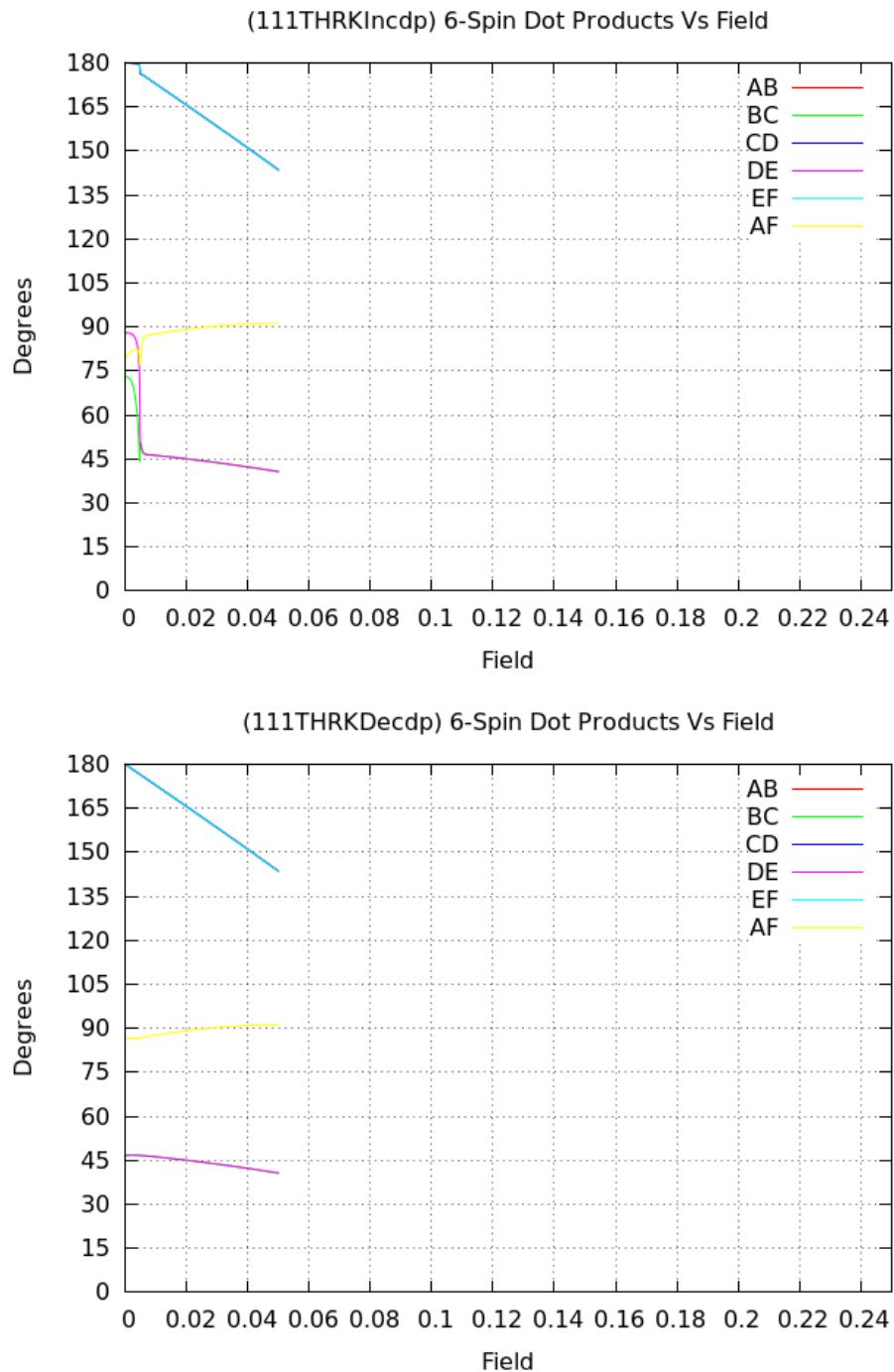


Figure 63: Dot products between the various characteristic spins for both increasing and decreasing fields.

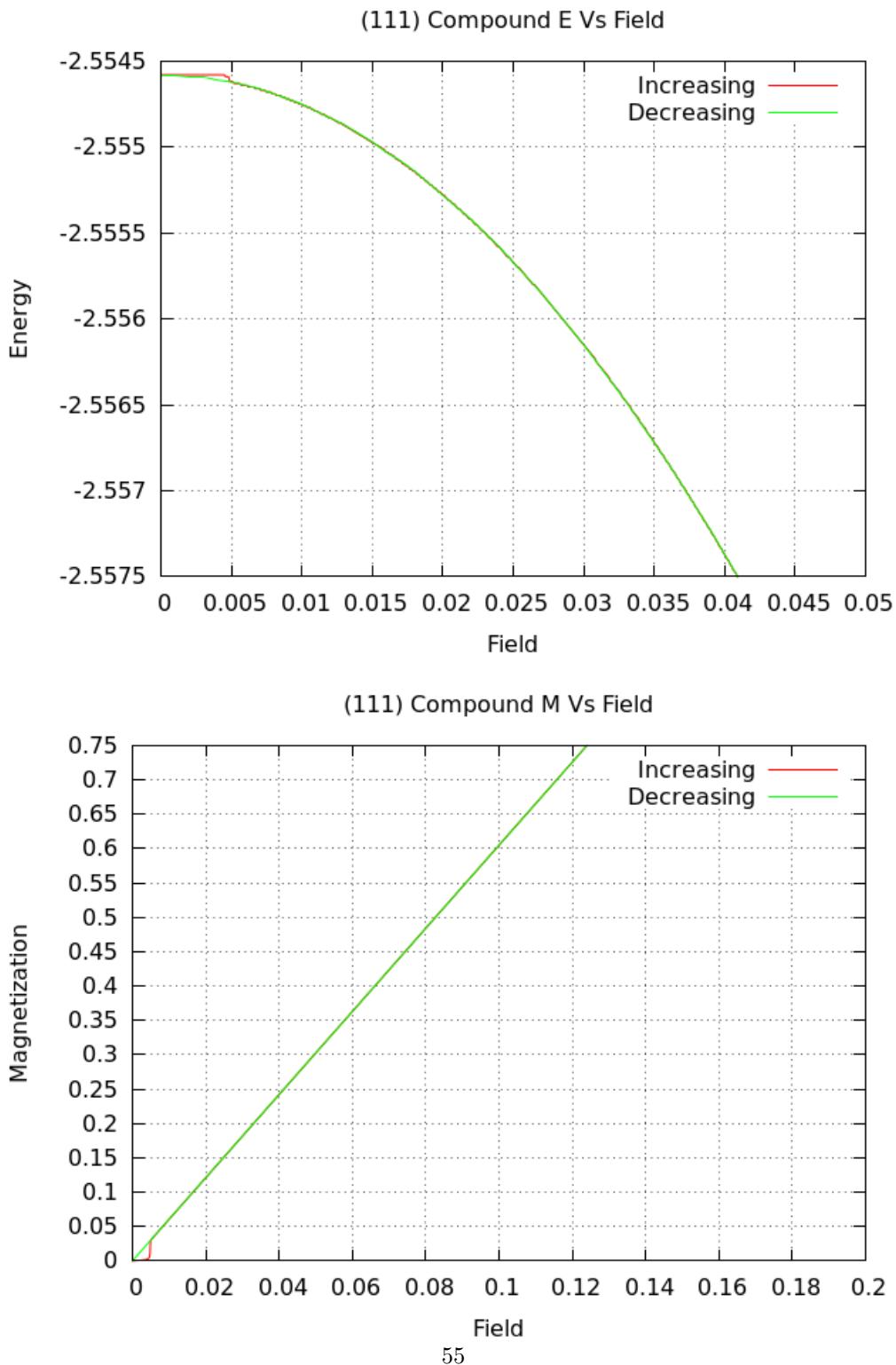


Figure 64: Composite graphs of energy and magnetization for both decreasing and increasing field magnitude. The magnetization actually plateaus at  $M=0.81$ , which is not shown here.

0.0500	6	0.045	6	0.04	6	0.035	6	0.03	6	0.025	6	0.02	6	0.015	6	0.01	6	0.005	6
0.0439	6	0.0449	6	0.0399	6	0.0349	6	0.0299	6	0.0249	6	0.0199	6	0.0149	6	0.0099	6	0.0049	6
0.0438	6	0.0448	6	0.0398	6	0.0348	6	0.0298	6	0.0248	6	0.0198	6	0.0148	6	0.0098	6	0.0048	6
0.0437	6	0.0447	6	0.0397	6	0.0347	6	0.0297	6	0.0247	6	0.0197	6	0.0147	6	0.0097	6	0.0047	6
0.0436	6	0.0446	6	0.0396	6	0.0346	6	0.0296	6	0.0246	6	0.0196	6	0.0146	6	0.0096	6	0.0046	6
0.0435	6	0.0445	6	0.0395	6	0.0345	6	0.0295	6	0.0245	6	0.0195	6	0.0145	6	0.0095	6	0.0045	6
0.0434	6	0.0444	6	0.0394	6	0.0344	6	0.0294	6	0.0244	6	0.0194	6	0.0144	6	0.0094	6	0.0044	6
0.0433	6	0.0443	6	0.0393	6	0.0343	6	0.0293	6	0.0243	6	0.0193	6	0.0143	6	0.0093	6	0.0043	6
0.0432	6	0.0442	6	0.0392	6	0.0342	6	0.0292	6	0.0242	6	0.0192	6	0.0142	6	0.0092	6	0.0042	6
0.0431	6	0.0441	6	0.0391	6	0.0341	6	0.0291	6	0.0241	6	0.0191	6	0.0141	6	0.0091	6	0.0041	6
0.0430	6	0.044	6	0.039	6	0.034	6	0.029	6	0.024	6	0.019	6	0.014	6	0.009	6	0.004	6
0.0429	6	0.0439	6	0.0389	6	0.0339	6	0.0289	6	0.0239	6	0.0189	6	0.0139	6	0.0089	6	0.0039	6
0.0428	6	0.0438	6	0.0388	6	0.0338	6	0.0288	6	0.0238	6	0.0188	6	0.0138	6	0.0088	6	0.0038	6
0.0427	6	0.0437	6	0.0387	6	0.0337	6	0.0287	6	0.0237	6	0.0187	6	0.0137	6	0.0087	6	0.0037	6
0.0426	6	0.0436	6	0.0386	6	0.0336	6	0.0286	6	0.0236	6	0.0166	6	0.0136	6	0.0066	6	0.0036	6
0.0425	6	0.0435	6	0.0385	6	0.0335	6	0.0285	6	0.0235	6	0.0185	6	0.0135	6	0.0085	6	0.0035	6
0.0424	6	0.0434	6	0.0384	6	0.0334	6	0.0284	6	0.0234	6	0.0184	6	0.0134	6	0.0084	6	0.0034	6
0.0423	6	0.0433	6	0.0383	6	0.0333	6	0.0283	6	0.0233	6	0.0183	6	0.0133	6	0.0083	6	0.0033	6
0.0422	6	0.0432	6	0.0382	6	0.0332	6	0.0282	6	0.0232	6	0.0182	6	0.0132	6	0.0082	6	0.0032	6
0.0421	6	0.0431	6	0.0381	6	0.0331	6	0.0281	6	0.0231	6	0.0181	6	0.0131	6	0.0081	6	0.0031	6
0.0420	6	0.043	6	0.038	6	0.033	6	0.028	6	0.023	6	0.018	6	0.013	6	0.008	6	0.003	6
0.0419	6	0.0429	6	0.0379	6	0.0329	6	0.0279	6	0.0229	6	0.0179	6	0.0129	6	0.0079	6	0.0029	6
0.0418	6	0.0428	6	0.0378	6	0.0328	6	0.0278	6	0.0228	6	0.0178	6	0.0128	6	0.0078	6	0.0028	6
0.0417	6	0.0427	6	0.0377	6	0.0327	6	0.0277	6	0.0227	6	0.0177	6	0.0127	6	0.0077	6	0.0027	6
0.0416	6	0.0426	6	0.0376	6	0.0326	6	0.0276	6	0.0226	6	0.0176	6	0.0126	6	0.0076	6	0.0026	6
0.0415	6	0.0425	6	0.0375	6	0.0325	6	0.0275	6	0.0225	6	0.0175	6	0.0125	6	0.0075	6	0.0025	6
0.0414	6	0.0424	6	0.0374	6	0.0324	6	0.0274	6	0.0224	6	0.0174	6	0.0124	6	0.0074	6	0.0024	6
0.0413	6	0.0423	6	0.0373	6	0.0323	6	0.0273	6	0.0223	6	0.0173	6	0.0123	6	0.0073	6	0.0023	6
0.0412	6	0.0422	6	0.0372	6	0.0322	6	0.0272	6	0.0222	6	0.0172	6	0.0122	6	0.0072	6	0.0022	6
0.0411	6	0.0421	6	0.0371	6	0.0321	6	0.0271	6	0.0221	6	0.0171	6	0.0121	6	0.0071	6	0.0021	6
0.0410	6	0.0420	6	0.037	6	0.032	6	0.027	6	0.022	6	0.017	6	0.012	6	0.007	6	0.002	6
0.0409	6	0.0419	6	0.0369	6	0.0319	6	0.0269	6	0.0219	6	0.0169	6	0.0119	6	0.0069	6	0.0019	6
0.0408	6	0.0418	6	0.0368	6	0.0318	6	0.0268	6	0.0218	6	0.0168	6	0.0118	6	0.0068	6	0.0018	6
0.0407	6	0.0417	6	0.0367	6	0.0317	6	0.0267	6	0.0217	6	0.0167	6	0.0117	6	0.0067	6	0.0017	6
0.0406	6	0.0416	6	0.0366	6	0.0316	6	0.0266	6	0.0216	6	0.0166	6	0.0116	6	0.0066	6	0.0016	6
0.0405	6	0.0415	6	0.0365	6	0.0315	6	0.0265	6	0.0215	6	0.0165	6	0.0115	6	0.0065	6	0.0015	6
0.0404	6	0.0414	6	0.0364	6	0.0314	6	0.0264	6	0.0214	6	0.0164	6	0.0114	6	0.0064	6	0.0014	6
0.0403	6	0.0413	6	0.0363	6	0.0313	6	0.0263	6	0.0213	6	0.0163	6	0.0113	6	0.0063	6	0.0013	6
0.0402	6	0.0412	6	0.0362	6	0.0312	6	0.0262	6	0.0212	6	0.0162	6	0.0112	6	0.0062	6	0.0012	6
0.0401	6	0.0411	6	0.0361	6	0.0311	6	0.0261	6	0.0211	6	0.0161	6	0.0111	6	0.0061	6	0.0011	6
0.0400	6	0.0410	6	0.036	6	0.031	6	0.026	6	0.021	6	0.016	6	0.011	6	0.006	6	0.001	6
0.0399	6	0.0409	6	0.0359	6	0.0309	6	0.0259	6	0.0209	6	0.0159	6	0.0109	6	0.0059	6	0.0009	6
0.0398	6	0.0408	6	0.0358	6	0.0308	6	0.0258	6	0.0208	6	0.0158	6	0.0108	6	0.0058	6	0.0008	7
0.0397	6	0.0407	6	0.0357	6	0.0307	6	0.0257	6	0.0207	6	0.0157	6	0.0107	6	0.0057	6	0.0007	6
0.0396	6	0.0406	6	0.0356	6	0.0306	6	0.0256	6	0.0206	6	0.0156	6	0.0106	6	0.0056	6	0.0006	6
0.0395	6	0.0405	6	0.0355	6	0.0305	6	0.0255	6	0.0205	6	0.0155	6	0.0105	6	0.0055	6	0.0005	6
0.0394	6	0.0404	6	0.0354	6	0.0304	6	0.0254	6	0.0204	6	0.0154	6	0.0104	6	0.0054	6	0.0004	6
0.0393	6	0.0403	6	0.0353	6	0.0303	6	0.0253	6	0.0203	6	0.0153	6	0.0103	6	0.0053	6	0.0003	6
0.0392	6	0.0402	6	0.0352	6	0.0302	6	0.0252	6	0.0202	6	0.0152	6	0.0102	6	0.0052	6	0.0002	7
0.0391	6	0.0401	6	0.0351	6	0.0301	6	0.0251	6	0.0201	6	0.0151	6	0.0101	6	0.0051	6	0.0001	6

Figure 65: Chart indicating the number of unique spins for decreasing the field in the 111 direction, when starting at a groundstate. No notable change in number of spins can be observed, except for the low field section when the number increases to 7 for two field values.

## 24 3K (111) Increasing Field, Random State

Similar to run 1, a transition to a planar state is observed at around 0.0037. This contrasts the transition field of 0.49 in the run starting from a ground state. This could be due to the fact the ground state that is initially generated at  $H=0$  is slightly different than that of the one used in run 1 and run 2. Maybe there is a relationship that tells us what field the transition will occur for a given theta and phi?

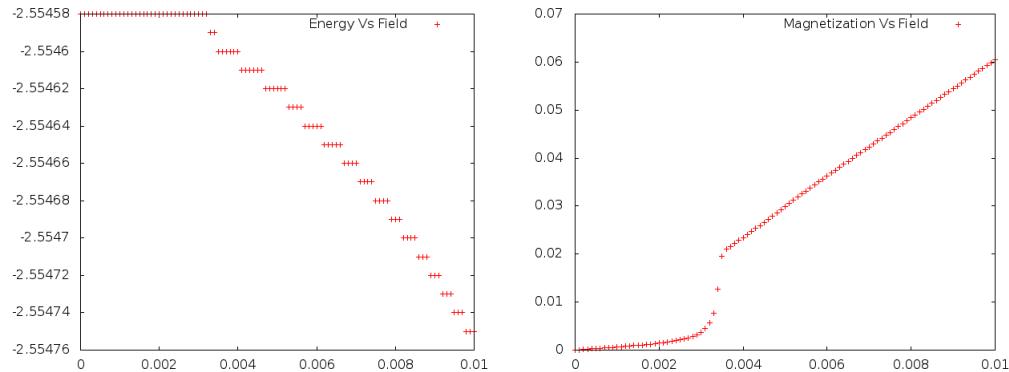


Figure 66: Energy vs increasing field and Magnetization versus increasing field

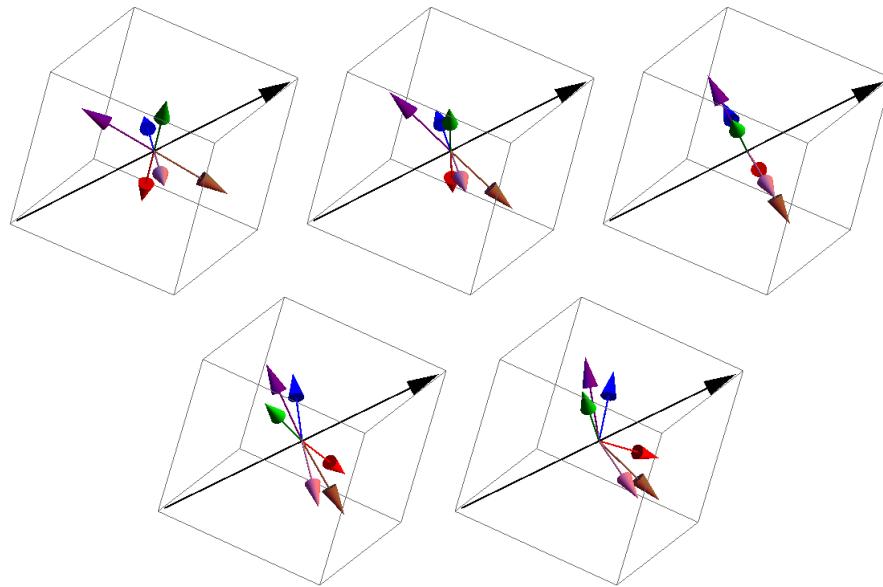


Figure 67: Snapshots of the 6 characteristic spins of the lattice at  $H=0.00$ ,  $0.0033$ ,  $0.0041$ ,  $0.0069$ , and  $0.0500$

0.0000	6	0.005	6	0.01	6	0.015	6	0.02	6	0.025	6	0.03	6	0.035	6	0.04	6	0.045	6
0.0001	6	0.0051	8	0.0101	6	0.0151	6	0.0201	6	0.0251	6	0.0301	6	0.0351	6	0.0401	6	0.0451	6
0.0002	6	0.0052	6	0.0102	6	0.0152	6	0.0202	6	0.0252	6	0.0302	6	0.0352	6	0.0402	6	0.0452	6
0.0003	6	0.0053	6	0.0103	6	0.0153	6	0.0203	6	0.0253	6	0.0303	6	0.0353	6	0.0403	6	0.0453	6
0.0004	6	0.0054	6	0.0104	6	0.0154	6	0.0204	6	0.0254	6	0.0304	6	0.0354	6	0.0404	6	0.0454	6
0.0005	6	0.0055	6	0.0105	6	0.0155	6	0.0205	6	0.0255	6	0.0305	6	0.0355	6	0.0405	6	0.0455	6
0.0006	6	0.0056	6	0.0106	6	0.0156	6	0.0206	6	0.0256	6	0.0306	6	0.0356	6	0.0406	6	0.0456	6
0.0007	6	0.0057	6	0.0107	6	0.0157	6	0.0207	6	0.0257	6	0.0307	6	0.0357	6	0.0407	6	0.0457	6
0.0008	6	0.0058	6	0.0108	6	0.0158	6	0.0208	6	0.0258	6	0.0308	6	0.0358	6	0.0408	6	0.0458	6
0.0009	6	0.0059	6	0.0109	6	0.0159	6	0.0209	6	0.0259	6	0.0309	6	0.0359	6	0.0409	6	0.0459	6
0.0010	6	0.006	6	0.011	6	0.016	6	0.021	6	0.026	6	0.031	6	0.036	6	0.041	6	0.046	6
0.0011	6	0.0061	6	0.0111	6	0.0161	6	0.0211	6	0.0261	6	0.0311	6	0.0361	6	0.0411	6	0.0461	6
0.0012	6	0.0062	6	0.0112	6	0.0162	6	0.0212	6	0.0262	6	0.0312	6	0.0362	6	0.0412	6	0.0462	6
0.0013	6	0.0063	6	0.0113	6	0.0163	6	0.0213	6	0.0263	6	0.0313	6	0.0363	6	0.0413	6	0.0463	6
0.0014	6	0.0064	6	0.0114	6	0.0164	6	0.0214	6	0.0264	6	0.0314	6	0.0364	6	0.0414	6	0.0464	6
0.0015	6	0.0065	6	0.0115	6	0.0165	6	0.0215	6	0.0265	6	0.0315	6	0.0365	6	0.0415	6	0.0465	6
0.0016	6	0.0066	6	0.0116	6	0.0166	6	0.0216	6	0.0266	6	0.0316	6	0.0366	6	0.0416	6	0.0466	6
0.0017	6	0.0067	6	0.0117	6	0.0167	6	0.0217	6	0.0267	6	0.0317	6	0.0367	6	0.0417	6	0.0467	6
0.0018	6	0.0068	6	0.0118	6	0.0168	6	0.0218	6	0.0268	6	0.0318	6	0.0368	6	0.0418	6	0.0468	6
0.0019	6	0.0069	6	0.0119	6	0.0169	6	0.0219	6	0.0269	6	0.0319	6	0.0369	6	0.0419	6	0.0469	6
0.0020	7	0.007	6	0.012	6	0.017	6	0.022	6	0.027	6	0.032	6	0.037	6	0.042	6	0.047	6
0.0021	6	0.0071	6	0.0121	6	0.0171	6	0.0221	6	0.0271	6	0.0321	6	0.0371	6	0.0421	6	0.0471	6
0.0022	6	0.0072	6	0.0122	6	0.0172	6	0.0222	6	0.0272	6	0.0322	6	0.0372	6	0.0422	6	0.0472	6
0.0023	6	0.0073	6	0.0123	6	0.0173	6	0.0223	6	0.0273	6	0.0323	6	0.0373	6	0.0423	6	0.0473	6
0.0024	6	0.0074	6	0.0124	6	0.0174	6	0.0224	6	0.0274	6	0.0324	6	0.0374	6	0.0424	6	0.0474	6
0.0025	6	0.0075	6	0.0125	6	0.0175	6	0.0225	6	0.0275	6	0.0325	6	0.0375	6	0.0425	6	0.0475	6
0.0026	6	0.0076	6	0.0126	6	0.0176	6	0.0226	6	0.0276	6	0.0326	6	0.0376	6	0.0426	6	0.0476	6
0.0027	7	0.0077	6	0.0127	6	0.0177	6	0.0227	6	0.0277	6	0.0327	6	0.0377	6	0.0427	6	0.0477	6
0.0028	7	0.0078	6	0.0128	6	0.0178	6	0.0228	6	0.0278	6	0.0328	6	0.0378	6	0.0428	6	0.0478	6
0.0029	6	0.0079	6	0.0129	6	0.0179	6	0.0229	6	0.0279	6	0.0329	6	0.0379	6	0.0429	6	0.0479	6
0.0030	6	0.008	6	0.013	6	0.018	6	0.023	6	0.028	6	0.033	6	0.038	6	0.043	6	0.048	6
0.0031	6	0.0081	6	0.0131	6	0.0181	6	0.0231	6	0.0281	6	0.0331	6	0.0381	6	0.0431	6	0.0481	6
0.0032	6	0.0082	6	0.0132	6	0.0182	6	0.0232	6	0.0282	6	0.0332	6	0.0382	6	0.0432	6	0.0482	6
0.0033	7	0.0083	6	0.0133	6	0.0183	6	0.0233	6	0.0283	6	0.0333	6	0.0383	6	0.0433	6	0.0483	6
0.0034	6	0.0084	6	0.0134	6	0.0184	6	0.0234	6	0.0284	6	0.0334	6	0.0384	6	0.0434	6	0.0484	6
0.0035	8	0.0085	6	0.0135	6	0.0185	6	0.0235	6	0.0285	6	0.0335	6	0.0385	6	0.0435	6	0.0485	6
0.0036	6	0.0086	6	0.0136	6	0.0186	6	0.0236	6	0.0286	6	0.0336	6	0.0386	6	0.0436	6	0.0486	6
0.0037	10	0.0087	6	0.0137	6	0.0187	6	0.0237	6	0.0287	6	0.0337	6	0.0387	6	0.0437	6	0.0487	6
0.0038	10	0.0088	6	0.0138	6	0.0188	6	0.0238	6	0.0288	6	0.0338	6	0.0388	6	0.0438	6	0.0488	6
0.0039	8	0.0089	6	0.0139	6	0.0189	6	0.0239	6	0.0289	6	0.0339	6	0.0389	6	0.0439	6	0.0489	6
0.0040	6	0.009	6	0.014	6	0.019	6	0.024	6	0.029	6	0.034	6	0.039	6	0.044	6	0.049	6
0.0041	6	0.0091	6	0.0141	6	0.0191	6	0.0241	6	0.0291	6	0.0341	6	0.0391	6	0.0441	6	0.0491	6
0.0042	6	0.0092	6	0.0142	6	0.0192	6	0.0242	6	0.0292	6	0.0342	6	0.0392	6	0.0442	6	0.0492	6
0.0043	6	0.0093	6	0.0143	6	0.0193	6	0.0243	6	0.0293	6	0.0343	6	0.0393	6	0.0443	6	0.0493	6
0.0044	8	0.0094	6	0.0144	6	0.0194	6	0.0244	6	0.0294	6	0.0344	6	0.0394	6	0.0444	6	0.0494	6
0.0045	6	0.0095	6	0.0145	6	0.0195	6	0.0245	6	0.0295	6	0.0345	6	0.0395	6	0.0445	6	0.0495	6
0.0046	6	0.0096	6	0.0146	6	0.0196	6	0.0246	6	0.0296	6	0.0346	6	0.0396	6	0.0446	6	0.0496	6
0.0047	6	0.0097	6	0.0147	6	0.0197	6	0.0247	6	0.0297	6	0.0347	6	0.0397	6	0.0447	6	0.0497	6
0.0048	7	0.0098	6	0.0148	6	0.0198	6	0.0248	6	0.0298	6	0.0348	6	0.0398	6	0.0448	6	0.0498	6
0.0049	6	0.0099	6	0.0149	6	0.0199	6	0.0249	6	0.0299	6	0.0349	6	0.0399	6	0.0449	6	0.0499	6

Figure 68: Number of unique spins within the lattice while increasing the field in the 111 direction after starting with a random initial configuration. The number of unique spins increases to 10 at  $H=0.0037$ .

## 25 3K (111) Decreasing Field, Random State

Very similar to decreasing the field in the 111 direction after starting with a ground state. However, it is different than decreasing the field in the 111 direction after starting with a random initial configuration with only 2000 steps. Here, 3000 steps were used and the resulting difference between this and the 2000 step case is the lack of a transition. It behaves exactly the same way if you were to start from a ground state.

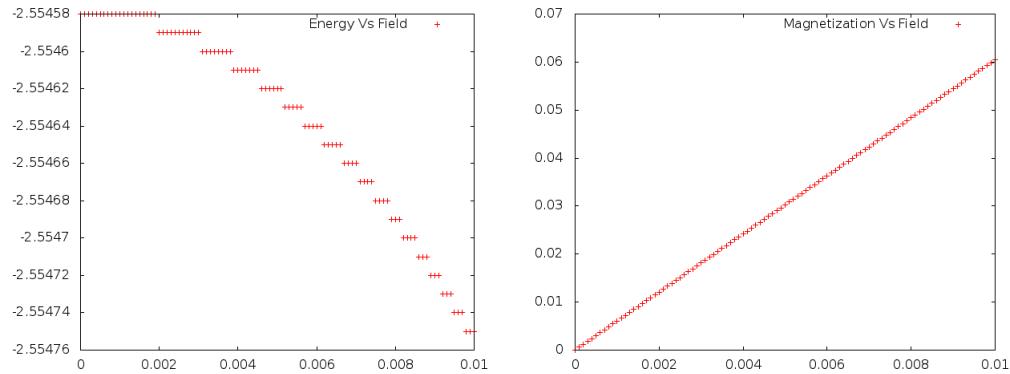


Figure 69: Energy vs decreasing field and Magnetization versus decreasing field

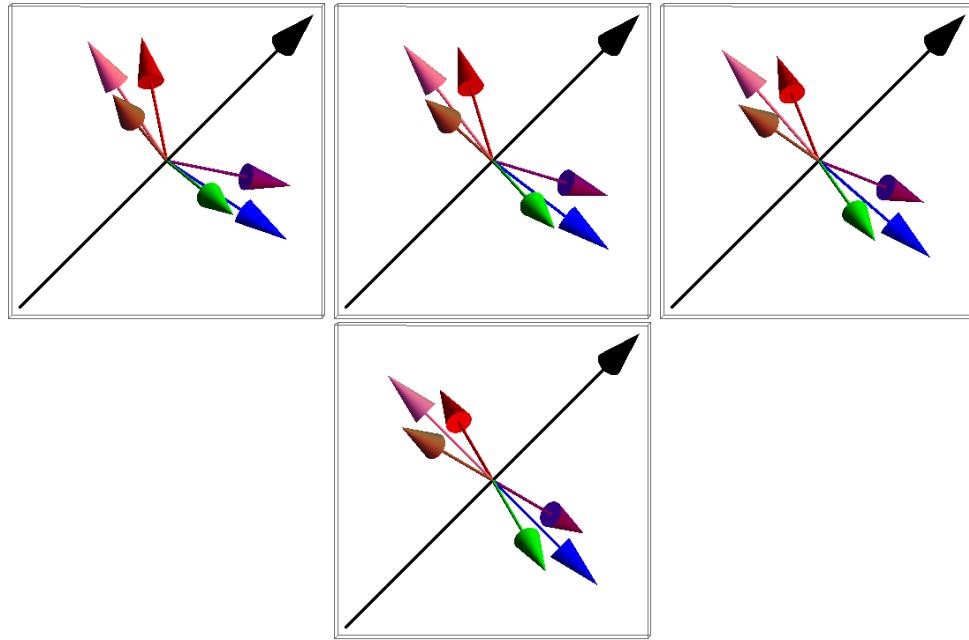


Figure 70: Snapshots of the 6 characteristic spins at  $H=0.05$ ,  $0.0329$ ,  $0.0176$ , and  $0$

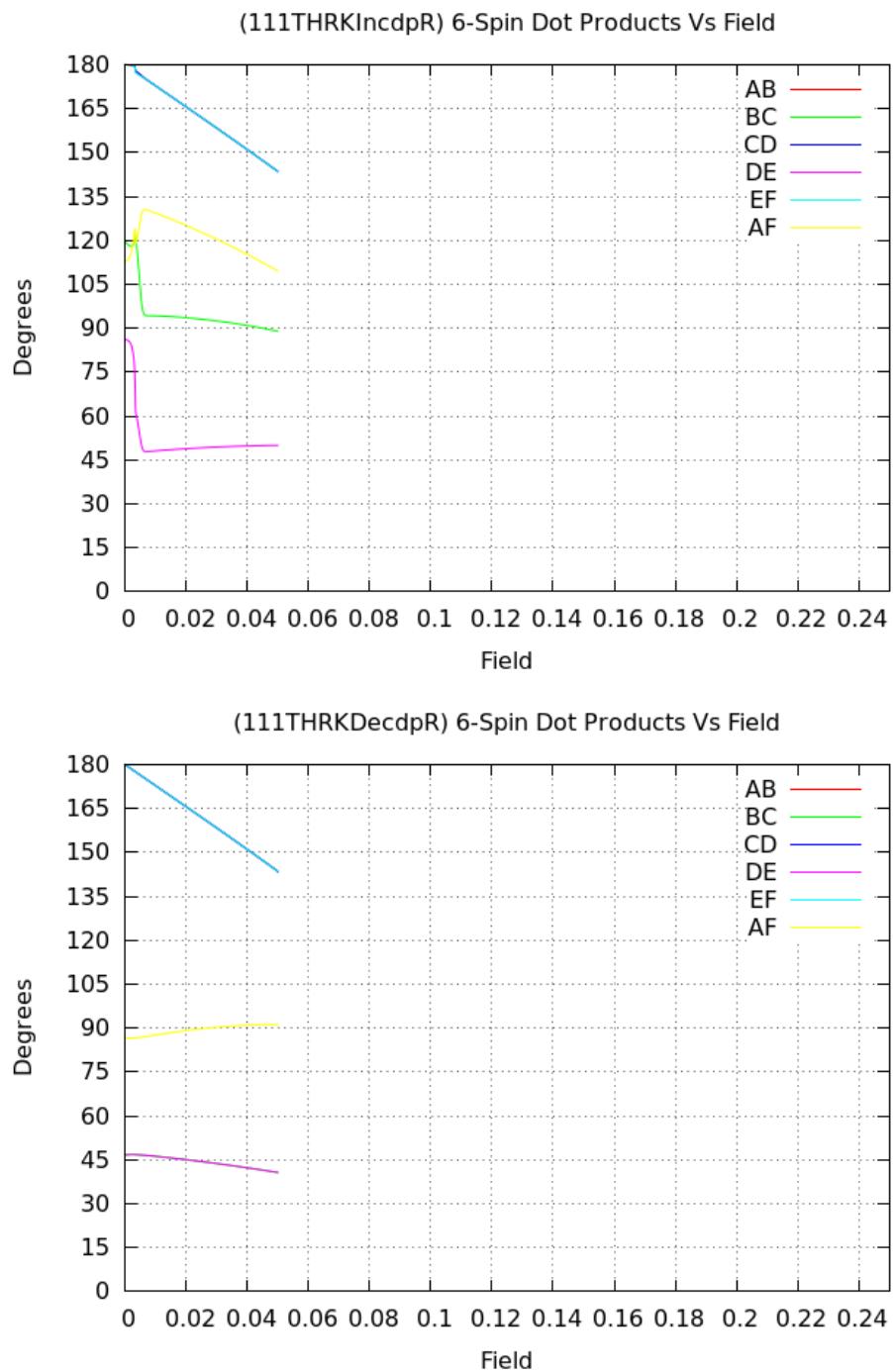


Figure 71: Dot products between the 6 characteristic spins.

0.0500	6	0.045	6	0.04	6	0.035	6	0.03	6	0.025	6	0.02	6	0.015	6	0.01	6	0.005	6
0.0499	6	0.0449	6	0.0399	6	0.0349	6	0.0299	6	0.0249	6	0.0199	6	0.0149	6	0.0099	6	0.0049	6
0.0498	6	0.0448	6	0.0398	6	0.0348	6	0.0298	6	0.0248	6	0.0198	6	0.0148	6	0.0098	6	0.0048	6
0.0497	6	0.0447	6	0.0397	6	0.0347	6	0.0297	6	0.0247	6	0.0197	6	0.0147	6	0.0097	6	0.0047	6
0.0496	6	0.0446	6	0.0396	6	0.0346	6	0.0296	6	0.0246	6	0.0196	6	0.0146	6	0.0096	6	0.0046	6
0.0495	6	0.0445	6	0.0395	6	0.0345	6	0.0295	6	0.0245	6	0.0195	6	0.0145	6	0.0095	6	0.0045	6
0.0494	6	0.0444	6	0.0394	6	0.0344	6	0.0294	6	0.0244	6	0.0194	6	0.0144	6	0.0094	6	0.0044	6
0.0493	6	0.0443	6	0.0393	6	0.0343	6	0.0293	6	0.0243	6	0.0193	6	0.0143	6	0.0093	6	0.0043	6
0.0492	6	0.0442	6	0.0392	6	0.0342	6	0.0292	6	0.0242	6	0.0192	6	0.0142	6	0.0092	6	0.0042	6
0.0491	6	0.0441	6	0.0391	6	0.0341	6	0.0291	6	0.0241	6	0.0191	6	0.0141	6	0.0091	6	0.0041	6
0.0490	6	0.044	6	0.039	6	0.034	6	0.029	6	0.024	6	0.019	6	0.014	6	0.009	6	0.004	6
0.0489	6	0.0439	6	0.0389	6	0.0339	6	0.0289	6	0.0239	6	0.0189	6	0.0139	6	0.0089	6	0.0039	6
0.0488	6	0.0438	6	0.0388	6	0.0338	6	0.0288	6	0.0238	6	0.0188	6	0.0138	6	0.0088	6	0.0038	6
0.0487	6	0.0437	6	0.0387	6	0.0337	6	0.0287	6	0.0237	6	0.0187	6	0.0137	6	0.0087	6	0.0037	6
0.0486	6	0.0436	6	0.0386	6	0.0336	6	0.0286	6	0.0236	6	0.0186	6	0.0136	6	0.0086	6	0.0036	6
0.0485	6	0.0435	6	0.0385	6	0.0335	6	0.0285	6	0.0235	6	0.0185	6	0.0135	6	0.0085	6	0.0035	6
0.0484	6	0.0434	6	0.0384	6	0.0334	6	0.0284	6	0.0234	6	0.0184	6	0.0134	6	0.0084	6	0.0034	6
0.0483	6	0.0433	6	0.0383	6	0.0333	6	0.0283	6	0.0233	6	0.0183	6	0.0133	6	0.0083	6	0.0033	6
0.0482	6	0.0432	6	0.0382	6	0.0332	6	0.0282	6	0.0232	6	0.0182	6	0.0132	6	0.0082	6	0.0032	6
0.0481	6	0.0431	6	0.0381	6	0.0331	6	0.0281	6	0.0231	6	0.0181	6	0.0131	6	0.0081	6	0.0031	6
0.0480	6	0.043	6	0.038	6	0.033	6	0.028	6	0.023	6	0.018	6	0.013	6	0.008	6	0.003	6
0.0479	6	0.0429	6	0.0379	6	0.0329	6	0.0279	6	0.0229	6	0.0179	6	0.0129	6	0.0079	6	0.0029	6
0.0478	6	0.0428	6	0.0378	6	0.0328	6	0.0278	6	0.0228	6	0.0178	6	0.0128	6	0.0078	6	0.0028	6
0.0477	6	0.0427	6	0.0377	6	0.0327	6	0.0277	6	0.0227	6	0.0177	6	0.0127	6	0.0077	6	0.0027	6
0.0476	6	0.0426	6	0.0376	6	0.0326	6	0.0276	6	0.0226	6	0.0176	6	0.0126	6	0.0076	6	0.0026	6
0.0475	6	0.0425	6	0.0375	6	0.0325	6	0.0275	6	0.0225	6	0.0175	6	0.0125	6	0.0075	6	0.0025	6
0.0474	6	0.0424	6	0.0374	6	0.0324	6	0.0274	6	0.0224	6	0.0174	6	0.0124	6	0.0074	6	0.0024	6
0.0473	6	0.0423	6	0.0373	6	0.0323	6	0.0273	6	0.0223	6	0.0173	6	0.0123	6	0.0073	6	0.0023	6
0.0472	6	0.0422	6	0.0372	6	0.0322	6	0.0272	6	0.0222	6	0.0172	6	0.0122	6	0.0072	6	0.0022	6
0.0471	6	0.0421	6	0.0371	6	0.0321	6	0.0271	6	0.0221	6	0.0171	6	0.0121	6	0.0071	6	0.0021	6
0.0470	6	0.042	6	0.037	6	0.032	6	0.027	6	0.022	6	0.017	6	0.012	6	0.007	6	0.002	6
0.0469	6	0.0419	6	0.0369	6	0.0319	6	0.0269	6	0.0219	6	0.0169	6	0.0119	6	0.0069	6	0.0019	6
0.0468	6	0.0418	6	0.0368	6	0.0318	6	0.0268	6	0.0218	6	0.0168	6	0.0118	6	0.0068	6	0.0018	6
0.0467	6	0.0417	6	0.0367	6	0.0317	6	0.0267	6	0.0217	6	0.0167	6	0.0117	6	0.0067	6	0.0017	6
0.0466	6	0.0416	6	0.0366	6	0.0316	6	0.0266	6	0.0216	6	0.0166	6	0.0116	6	0.0066	6	0.0016	6
0.0465	6	0.0415	6	0.0365	6	0.0315	6	0.0265	6	0.0215	6	0.0165	6	0.0115	6	0.0065	6	0.0015	6
0.0464	6	0.0414	6	0.0364	6	0.0314	6	0.0264	6	0.0214	6	0.0164	6	0.0114	6	0.0064	6	0.0014	6
0.0463	6	0.0413	6	0.0363	6	0.0313	6	0.0263	6	0.0213	6	0.0163	6	0.0113	6	0.0063	6	0.0013	6
0.0462	6	0.0412	6	0.0362	6	0.0312	6	0.0262	6	0.0212	6	0.0162	6	0.0112	6	0.0062	6	0.0012	6
0.0461	6	0.0411	6	0.0361	6	0.0311	6	0.0261	6	0.0211	6	0.0161	6	0.0111	6	0.0061	6	0.0011	6
0.0460	6	0.041	6	0.036	6	0.031	6	0.026	6	0.021	6	0.016	6	0.011	6	0.006	6	0.001	6
0.0459	6	0.0409	6	0.0359	6	0.0309	6	0.0259	6	0.0209	6	0.0159	6	0.0109	6	0.0059	6	0.0009	6
0.0458	6	0.0408	6	0.0358	6	0.0308	6	0.0258	6	0.0208	6	0.0158	6	0.0108	6	0.0058	6	0.0008	7
0.0457	6	0.0407	6	0.0357	6	0.0307	6	0.0257	6	0.0207	6	0.0157	6	0.0107	6	0.0057	6	0.0007	6
0.0456	6	0.0406	6	0.0356	6	0.0306	6	0.0256	6	0.0206	6	0.0156	6	0.0106	6	0.0056	6	0.0006	6
0.0455	6	0.0405	6	0.0355	6	0.0305	6	0.0255	6	0.0205	6	0.0155	6	0.0105	6	0.0055	6	0.0005	6
0.0454	6	0.0404	6	0.0354	6	0.0304	6	0.0254	6	0.0204	6	0.0154	6	0.0104	6	0.0054	6	0.0004	6
0.0453	6	0.0403	6	0.0353	6	0.0303	6	0.0253	6	0.0203	6	0.0153	6	0.0103	6	0.0053	6	0.0003	6
0.0452	6	0.0402	6	0.0352	6	0.0302	6	0.0252	6	0.0202	6	0.0152	6	0.0102	6	0.0052	6	0.0002	7
0.0451	6	0.0401	6	0.0351	6	0.0301	6	0.0251	6	0.0201	6	0.0151	6	0.0101	6	0.0051	6	0.0001	6

Figure 72: Number of unique spins within the lattice while decreasing the field in the 111 direction after starting from an initially random configuration.

## 26 Saturation of the Lattice

Using the same groundstate as used in all simulations, 7 simulations were run with differing field directions. The field was increased up until saturating the lattice. 001 and 010 both have identical magnetization curves, as do 011 and 101. However, 100 differs from 001 and 010, and 110 differs from 011 and 101, which is unexpected. When using the 111 field direction, saturation occurs at a field that is higher than the saturation fields of any other simulations.

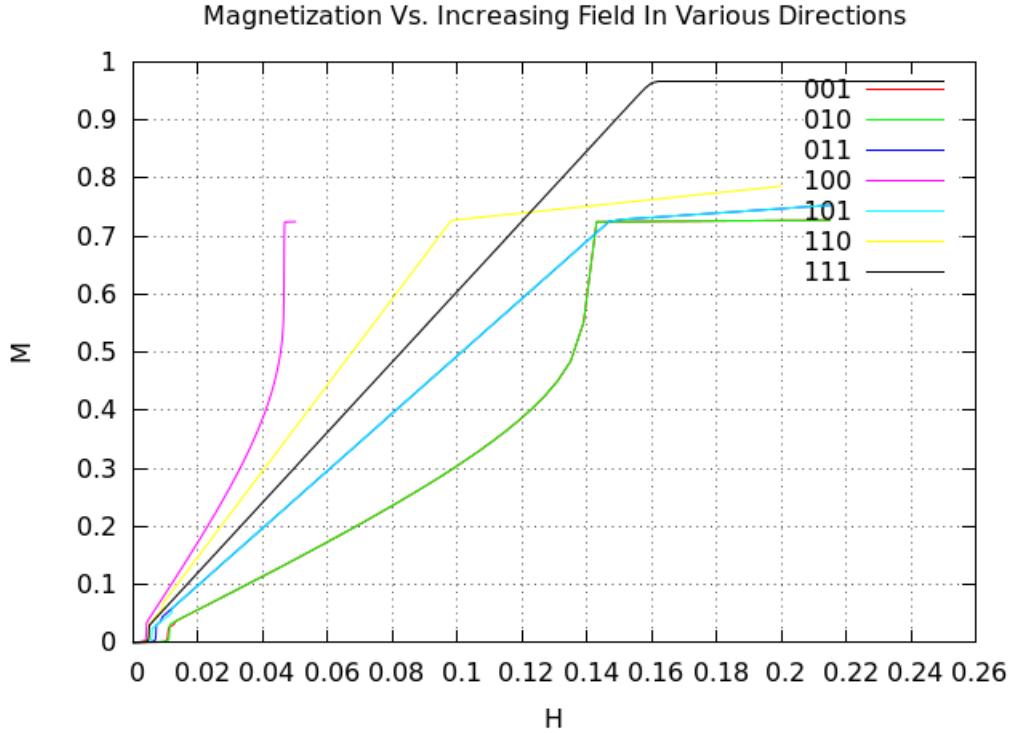


Figure 73: Magnetization curves starting with the same ground state and subjected to fields of various directions

## 27 Effect of Starting State on Switching Field (111)

To determine the effect the starting state has on when the lattice transitions to a planar state, 97 pairs of theta and phi were generated. These pairs were not randomly generated, but were generated by incrementing theta and phi through a for loop. While the contour plot gives the impression that pairs of theta and phi were generated from the forbidden zone and underwent a transition, this is simply the result of interpolation by Mathematica. The field used was along the 111 axis.

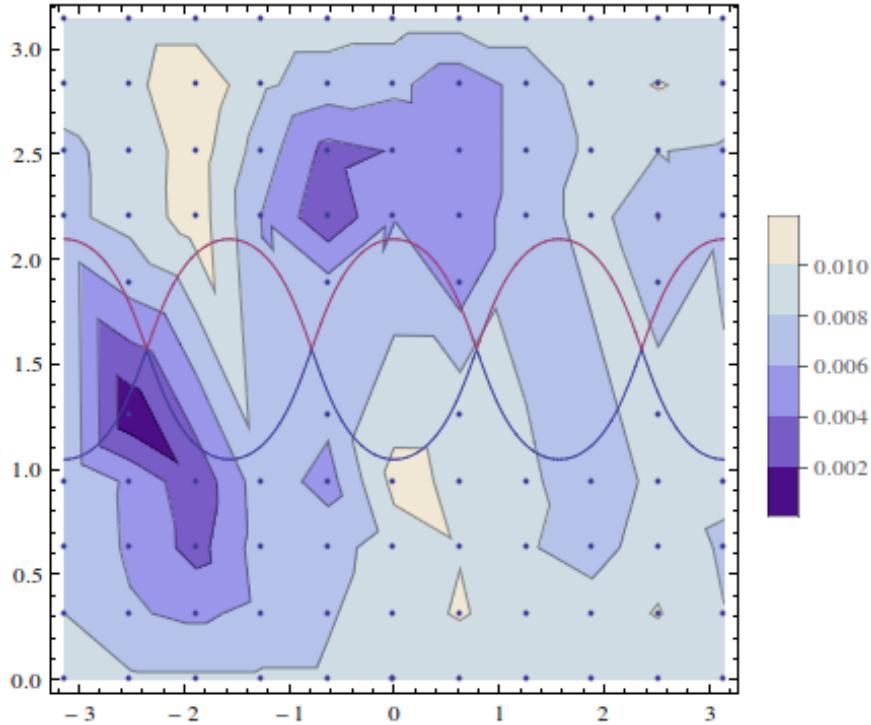


Figure 74: Contour plot indicating what pairs of theta and phi generate groundstates that transition sooner than others in the presence of the 111 field direction. The values in the legend are the magnitudes of the fields at which a point of inflection occurred and resulted in a transition. The reason why some states transition sooner than others could just be from the fact that certain states are already closer to the planar state at zero field. So there's less change in the spin components required to transition to the planar state. For example, at the darkest region there was a pair of theta and phi that gave rise to a starting state that I think was already planar. So in a way it had already transitioned at zero field. The region surrounding this point also transitions fairly quickly in comparison to most of the plane. I think there might be something special about the ground state that had already transitioned at zero field; that is, its theta and phi might describe 1 or more post-transition planar states.

## 28 Effect of Field Direction on Switching Field

To observe the effect of field direction on the switching field for a particular ground state (the same groundstate used in all groundstate simulations), the z-component of the applied magnetic field was varied for 20 different simulations. The result is that the switching field seems to change with a linear relationship with respect to the changing z-component. The switching field was approximated by finding the point of inflection for each of the magnetization curves.

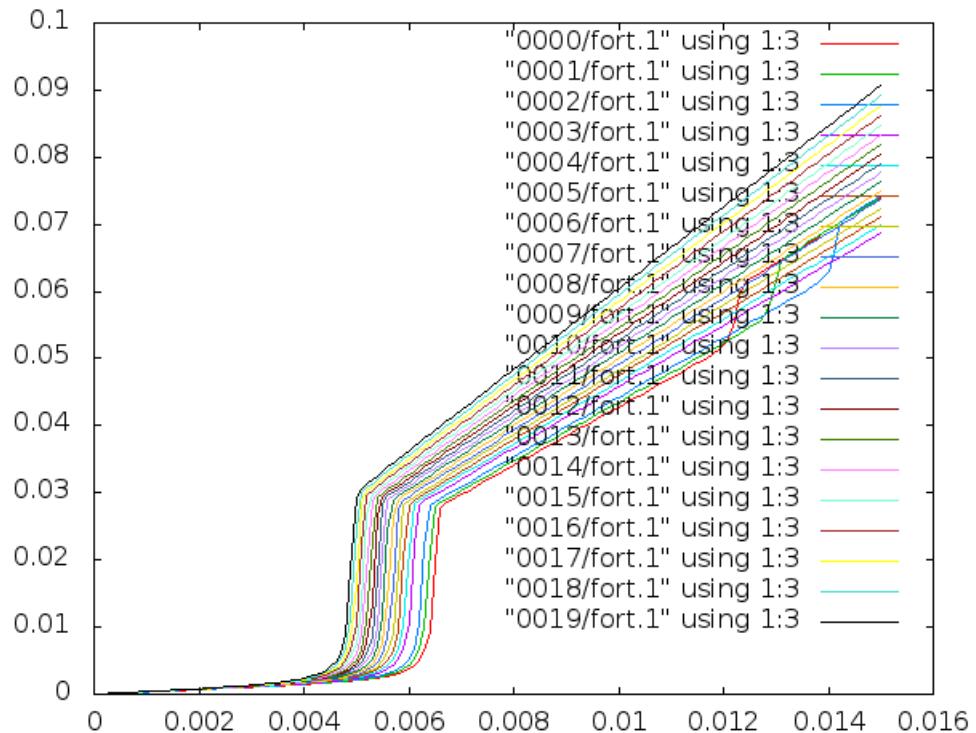


Figure 75: Magnetization curves for each simulation. The z-component was varied by increments of 5 percent for each simulation

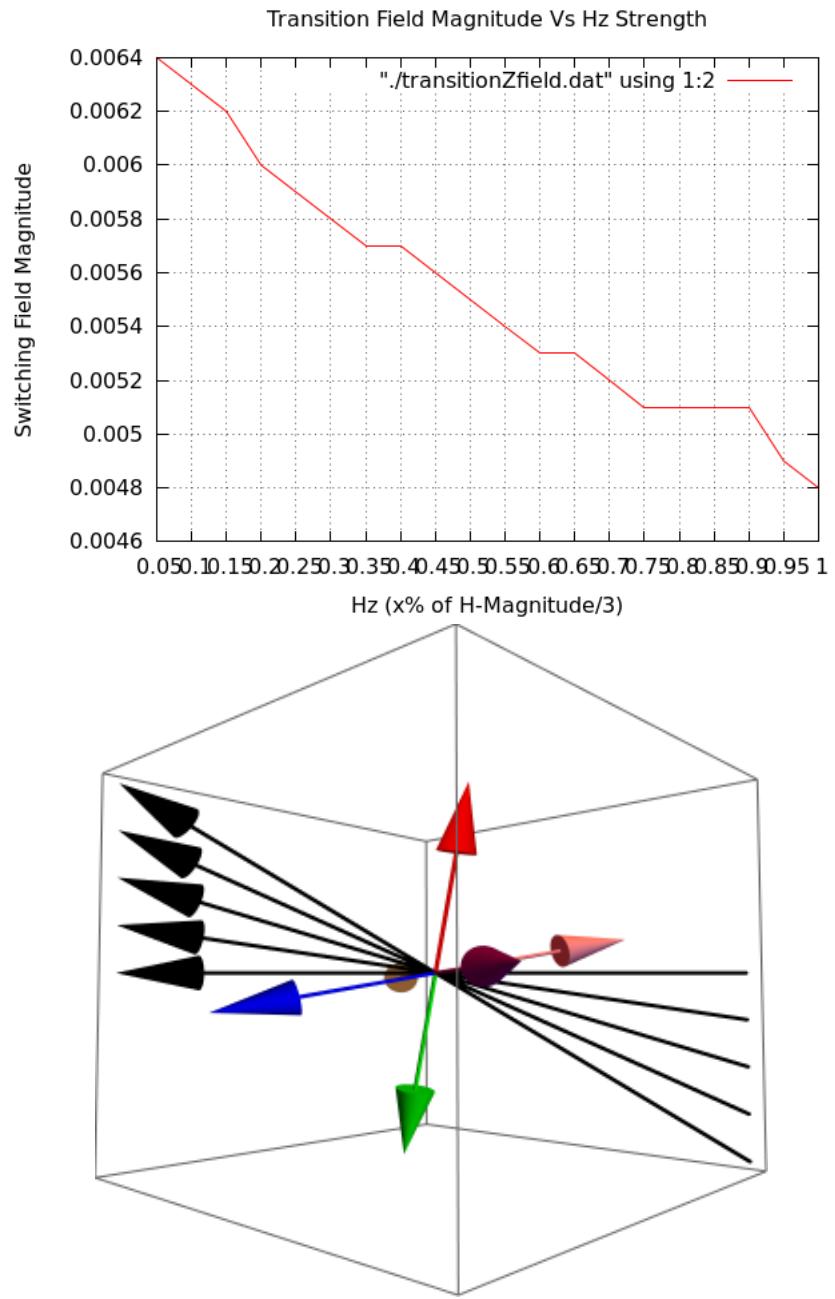


Figure 76: Switching field magnitude as a function of z-component strength. A visualization depicting how the field was changed for each independent simulation is also shown.

## 29 Reduction of Degeneracy By Application of Field

To gain insight on the possibility of being able to reduce the degree of the degeneracy by application of a field, 21 initially random spin configurations were created and subjected to an increasing magnetic field in the 111 direction. Once they surpassed the transition point, the field was then decreased to zero. What was observed was that each state fell into 1 of 6 possible zero field configurations, illustrated below:

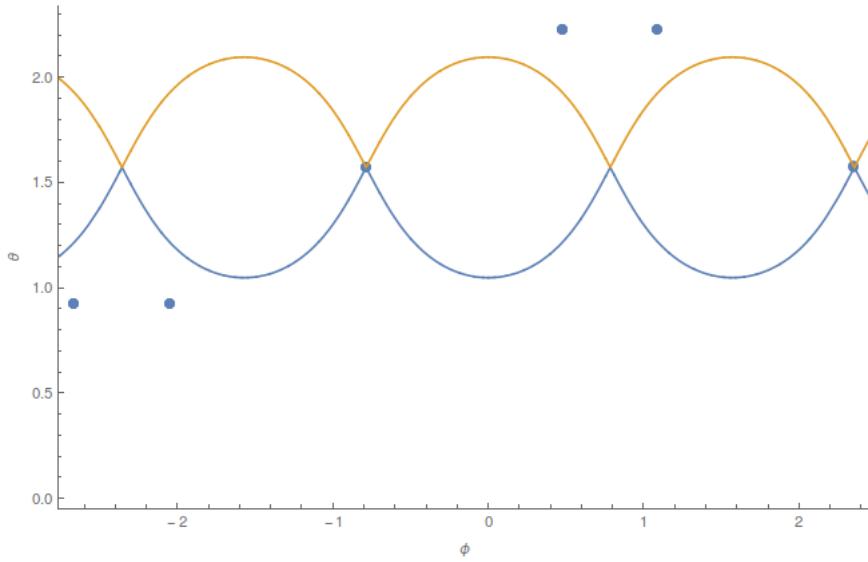


Figure 77: Depiction of what pairs of theta and phi characterize the groundstates after decreasing the field to zero for the 111 field.

Theta	Phi	Percent
127.26	27.3352	28.57
52.7912	-117.385	14.29
52.8063	-152.599	19.05
127.249	62.6494	14.29
90.02	-45.016	14.29
90.1097	135	9.52

Table 1: The 6 pairs of characteristic ground state angles describing the 6 possible states that result after decreasing the 111 field.

It can also be noted that when decreasing the field, after transitioning, for both the 010 and 111 field directions, after starting from the same ground state, the characteristic angles were the same: 52.7815, -117.275 (010), 52.1404 -116.39 (111).

## 30 Concluding Remarks

There are several things that can be noted through this pdf, and I'll try to summarize them here:

1. The field magnitude at which the lattice undergoes a transition is dependent on the starting spin configuration
2. The field magnitude at which the lattice undergoes a transition is dependent on the field direction.
3. The continuous degeneracy collapses to a collection of likely 6 possible groundstates, regardless of initial configuration.

Some starting states result in a transition sooner than others, which can be seen in the contour plot. This makes sense since some starting configurations are probably “closer” to the planar state (or one of 6 planar states) and require less field to bring them to their pending planar state.

By changing the field direction, transitions can be made to occur earlier for a particular ground state configuration. What has yet to be determined, however, is whether the change in field will have any effect on the types of planar states that the spin configuration turns into once the field is decreased to zero.

To gain some more insight on how the ground state degeneracy changes as a result of being subject to a field, I'm planning as of now to do the following:

Analyze recently completed simulations that involved generating 20 initially random configurations for each of the field directions used in this pdf. By increasing the field, then decreasing the field for each simulation, I will determine what effect changing the field direction has on collapsing the continuous degeneracy. Will it change the possible ground state combinations? Is the possible ground state combinations the same regardless of field direction?

Finally, there are several long term goals that should be addressed at some point in the future, and are as follows:

1. Analytical description of how spins change before transitioning, or how the Byron-Andrew relations change with respect to changing field prior to transitioning.
2. An analytical description of when the lattice will undergo a transition for a given starting configuration and field direction
3. A description of how the spins change after transitioning, but prior to the lattice becoming saturated. This should be fairly straightforward since there is a linear relationship between the spin component and field magnitude for a field of some direction.
4. A description that predicts when saturation will occur for a particular field direction.
5. Determining how the spins will change after becoming saturated. This should also be straight forward, since the change is linear.
6. Why aren't 100, 010, 001 magnetization curves all the same? Furthermore, why aren't 011, 101, and 110 magnetization curves all the same?