

Continuous Degeneracy and Magnetization Process in the 3D FCC Kagome Lattice with the Dipole-Dipole Interaction

by

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Department of Physics

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Abstract

Results are presented on analytic and computational analyses of the spin states associated with ABC stacked kagome planes of magnetic ions with only long-range dipole-dipole interactions. Extending previous work on the 2D kagome system, where six-fold discrete degeneracy of the ground state was revealed [1], we show that the 3D FCC kagome lattice exhibits a continuous degeneracy characterized by just six sub-lattice spin vectors and two spherical angles. Thermal fluctuations are shown to lift this degeneracy in an order-by-disorder process. Degaussing the lattice with a magnetic field applied along directions of high symmetry also results in lifting the continuous degeneracy to a subset of states from the original set of ground states, characterized by a single parameter. This lattice type is a model for the magnetic Mn ions in IrMn₃, the most popular compound used as the antiferromagnetic pinning layer in hard-drive spin valve structures [2]. Analysis of these spin states is relevant for a deeper understanding of magnetic and thermal stability at surfaces and in thin films of IrMn₃.

Acknowledgements

At a minimum you must acknowledge the funding sources for your work.

Table of Contents

Abstract	ii
Acknowledgments	iii
Table of Contents	v
List of Tables	vi
List of Figures	vii
List of Abbreviations and Symbols	vii
1 Introduction (can be a more descriptive title)	1
1.1 A section	1
1.1.1 A subsection about getting organized	1
1.1.2 Scope	2
1.2 Another section	2
1.2.1 Some technical details	2
2 Methods	4
2.1 Substrate preparation	4
2.1.1 Lots of chemicals	5

2.2	Atomic Force Microscopy	5
3	Another chapter	6
3.1	Ground State Degeneracy	6
3.1.1	Visualization of the Ground State	11
3.1.2	Planar Ground States	13
A	Extra spectra	15
A.1	What should go in an appendix?	15
	Bibliography	15

List of Tables

- 2.1 Note how this caption is at the top of the table. Also, note that the
caption in the List of Tables doesn't include the reference number. . . 4

List of Figures

2.1	Schematic of an atomic force microscope. Note that the size of the text in the figure is comparable to the size of the main text. Reproduced under Public Domain from Wikimedia Commons	5
3.1	A view down the $\langle 1,1,1 \rangle$ axis of a 3D FCC lattice with six sub-lattice spin vectors.	7
3.2	A plane that contains points that allow the construction of valid ground states.	9
3.3	One section of the original degeneracy plane that is equivalent to all other sections of the plane due to symmetry operations.	10
3.4	The six sublattice spins conjoined at their ends for clarity and illustration. The vector denoting $\langle 1,1,1 \rangle$ axis of symmetry is illustrated in black	11
3.5	A contour plot of volume of a parallelopiped formed by a spin configuration with respect to θ and ϕ	12
3.6	View 1	14
3.7	View 2	14
3.8	View 3	14
3.9	View 4	14

List of Abbreviations and Symbols

If you don't have a list of abbreviations, then you don't need to include this file and you can comment out the corresponding lines in your main .tex file. For example, if this file just defined a couple of terms such as AFM, then you wouldn't necessarily need this.

If you do have abbreviations to define, then you will probably set them up in a table like this:

E	energy
\vec{E}	electric field
EFMS	Erika

Chapter 1

Introduction (can be a more descriptive title)

1.1 A section

Your first step in using this template should be to rename the folder and main .tex file to something involving your name. That will help me to keep track of the various theses I'm reading!

1.1.1 A subsection about getting organized

Then start creating an outline for your thesis. If you already have chapters written as papers, perhaps you should be using the “MUN_Thesis_multiple_bibliographies” template.

To create the outline, create the chapters and write in all of the sections, subsections, etc. Then send that file to me so that I can look it over. This is particularly important for the introduction or background chapter. If we agree on the scope of your thesis up front, you will save yourself time later.

1.1.2 Scope

The main purpose of the first section is to provide the context for your work. What have other people done in this area, with these techniques? What background information does a somewhat general reader (*e.g.* chemist just starting a graduate program) need to know in order to appreciate and understand your work?

1.2 Another section

As you write your thesis, be sure to use labels and references for your tables, figures, equations, chapters, etc. This is another important aspect of getting organized, a topic which was discussed in Section 1.1.1. Be sure to pick unique labels. For example, “raman” or “afm” are probably not good labels, since you will probably have multiple figures, tables, equations, and sections which could carry those labels. Your whole thesis, including material in, for example, Appendix A, will have one common list of labels.

Note the pretty quotes around raman and the not-so-pretty quotes around afm. See the .tex file to know how to do this.

1.2.1 Some technical details

Pretty much all equations should be set off and numbered rather than included inline. The Tabor coefficient, μ , can be used to determine whether material deformation should be taken into account. [?]

$$\mu = \left[\frac{R(\Delta\gamma)^2}{E^*2\sigma^3} \right]^{1/3} \quad (1.1)$$

where R is the indenter tip radius, $\Delta\gamma$ is the work of adhesion, σ is the separation, and E^* is defined as

$$\frac{1}{E^*} = \frac{1 - \nu_{\text{tip}}^2}{E_{\text{tip}}} + \frac{1 - \nu_{\text{sample}}^2}{E_{\text{sample}}} \quad (1.2)$$

ν_{tip} is....

Note that the equations are part of a paragraph. Check how this is done in the .tex file, by not leaving blank lines before or after the equation. Also, note that the font used in the text for the symbols is the same as that used in the equation, and that text in the equation doesn't need to be in math mode.

Chapter 2

Methods

2.1 Substrate preparation

This is a good chapter to write continuously throughout your degree program. It will be easier to write up a procedure while it's fresh in your mind, and that way you won't be hunting down an instrument model or consumables supplier later.

If you are varying several parameters in your procedure, you may want to tabulate your different combinations. Table 2.1 summarizes ice cream texture characteristics used by McGhee et al [?].

Table 2.1: Note how this caption is at the top of the table. Also, note that the caption in the List of Tables doesn't include the reference number. [?].

Characteristic	Mean value
Icy	4.63
Crumbly	4.75
Fluffy	4.58
Gummy	4.71
Sandy	4.58
Soggy	4.29
Weak body	3.92

2.1.1 Lots of chemicals

I used K_2HPO_4 , $\text{KH}_2\text{PO}_4 \cdot 2\text{H}_2\text{O}$, and other salts containing PO_4^{3-} ions. Best of all, I didn't write out those chemical formula by hand using subscripts and superscripts. See the .tex file to find out how!

2.2 Atomic Force Microscopy

A picture is worth a thousand words! If you are creating your own schematics, consider using a program which will save images in a precise and generally readable format such as SVG. Inkscape will do that for you and is open source.

There are many public domain and other freely reproducible images available on the Wikimedia Commons. You can also easily get permission to reuse a figure from most journals through RightsLink.

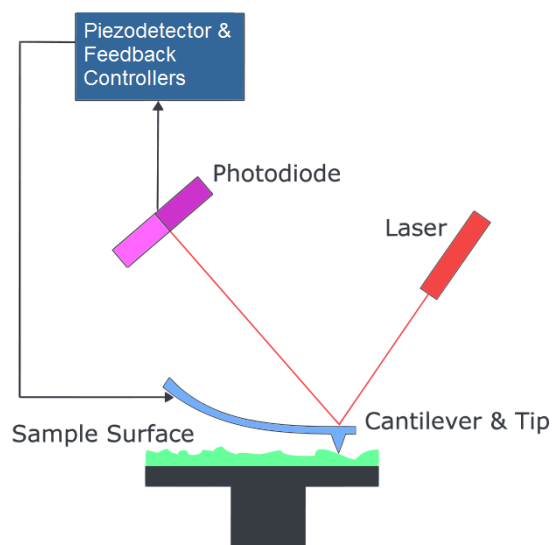


Figure 2.1: Schematic of an atomic force microscope. Note that the size of the text in the figure is comparable to the size of the main text. Reproduced under Public Domain from Wikimedia Commons

Chapter 3

Another chapter

3.1 Ground State Degeneracy

In this chapter results of simulations on the dipolar kagome lattice are presented. EFM simulations reveal zero-temperature states lacking domain walls that consist of 3 spins and their negatives. Every ground state obtained through the EFM simulation exhibits a three-sublattice structure with one spin and its negative for each sublattice. The spins alternate in direction along the $[1,1,1]$ direction.

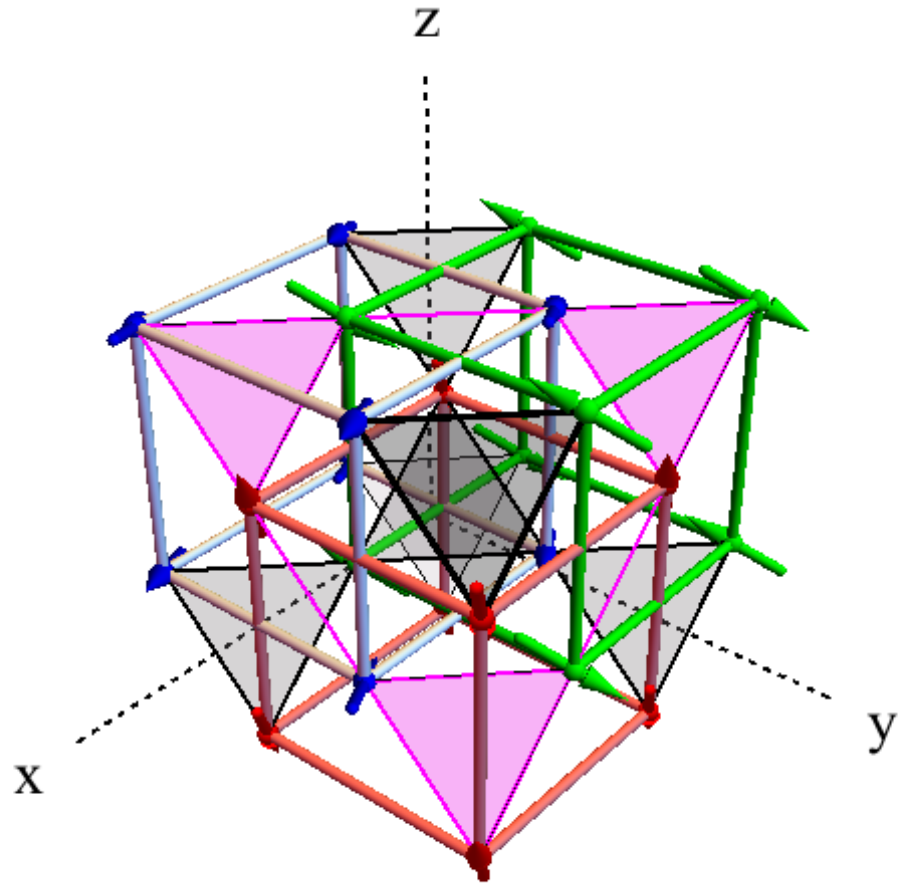


Figure 3.1: A view down the $\langle 1,1,1 \rangle$ axis of a 3D FCC lattice with six sub-lattice spin vectors.

Every ground state configuration obtained through the EFM simulation is characterized by the following set of equations:

$$\alpha = \sin \theta \cos \phi \quad (3.1)$$

$$\beta = \sin \theta \sin \phi \quad (3.2)$$

$$\chi = \cos \theta \quad (3.3)$$

$$\delta = (2a^2 - 1)/2c \quad (3.4)$$

$$\epsilon = \sqrt{(1 - a^2 - d^2)} \quad (3.5)$$

This set of equations acts as elementary building blocks for the components of the spin vectors that exist in the dipolar kagome ground state. The spin vectors may be constructed with this set of equations using the following configuration.

$$\vec{a} = (\alpha, \beta, \chi)$$

$$\vec{b} = (\delta, \epsilon, -\alpha)$$

$$\vec{c} = (-\epsilon, -\chi - \delta, \beta)$$

$$\vec{d} = -\vec{a}$$

$$\vec{e} = -\vec{b}$$

$$\vec{f} = -\vec{c}$$

The set of all possible ground states is therefore characterizable in terms of two parameters: θ and ϕ . Any θ and ϕ gives rise to an acceptable ground state of the same energy for a particular lattice size, with the exception of a subset of

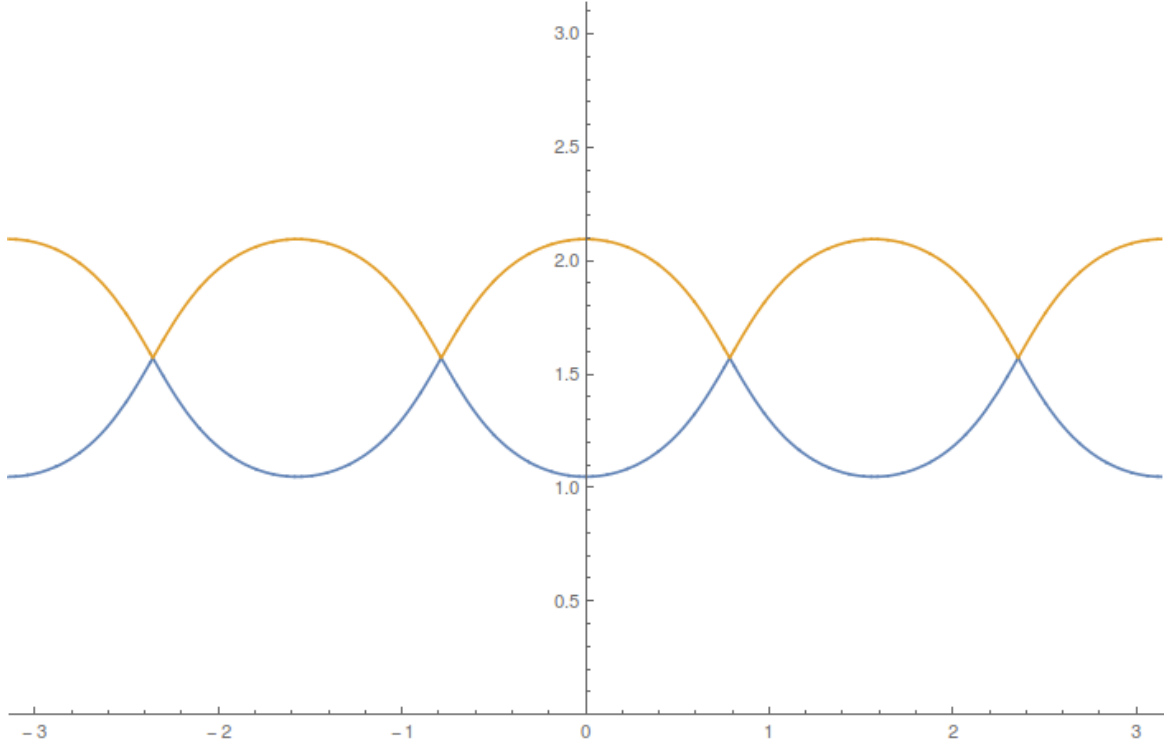


Figure 3.2: A plane that contains points that allow the construction of valid ground states.

angles that results in imaginary values for the spin components or undefined division by zero.

Any theta and phi will give rise to a valid ground state of the same energy with the exception of those pairs of theta and phi that lie within the bound region of the graph. Within the bound region of the graph, $e = \sqrt{1-a^2-d^2} \in \mathbb{C}$. At each node of each bound area, $d = (2a^2-1)/2c \rightarrow \pm 0/0$. Therefore, any choice of theta and phi outside of this region will give rise to a valid ground state of the same energy.

It is possible to reduce the size of this graph to 1/16 the size by showing that a state in each portion of the graph is relatable to an analogous state in the other portions of the graph via symmetry operations.

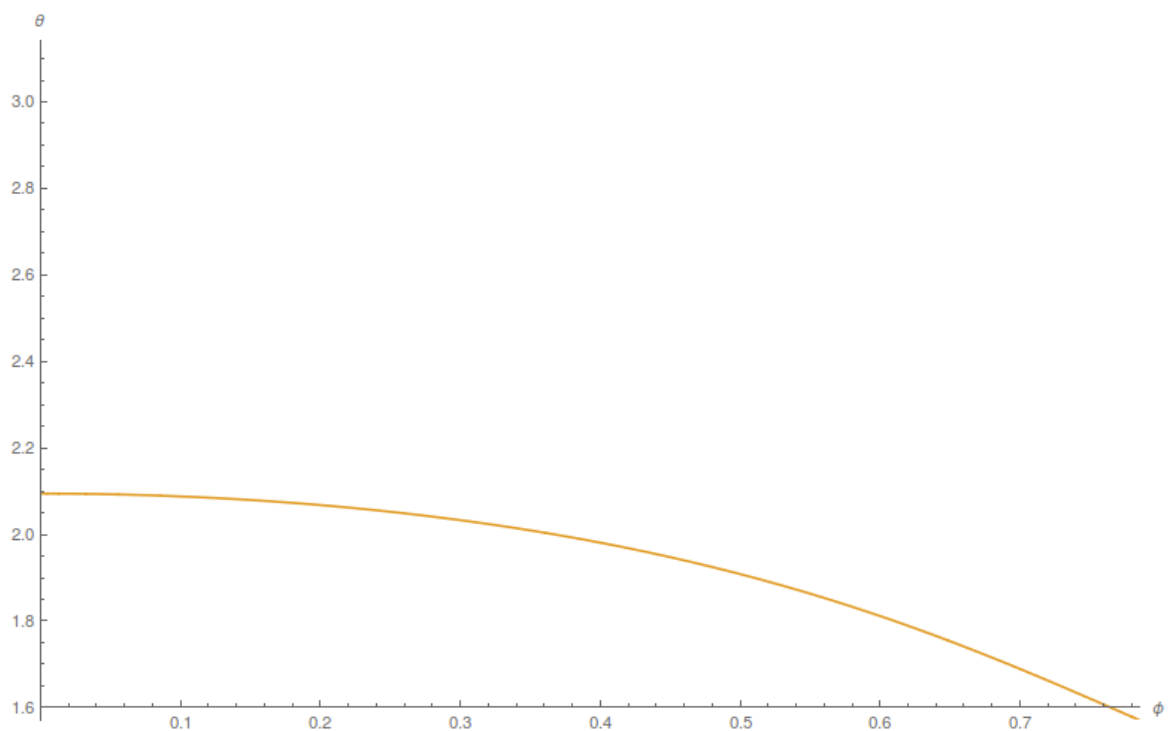


Figure 3.3: One section of the original degeneracy plane that is equivalent to all other sections of the plane due to symmetry operations.

3.1.1 Visualization of the Ground State

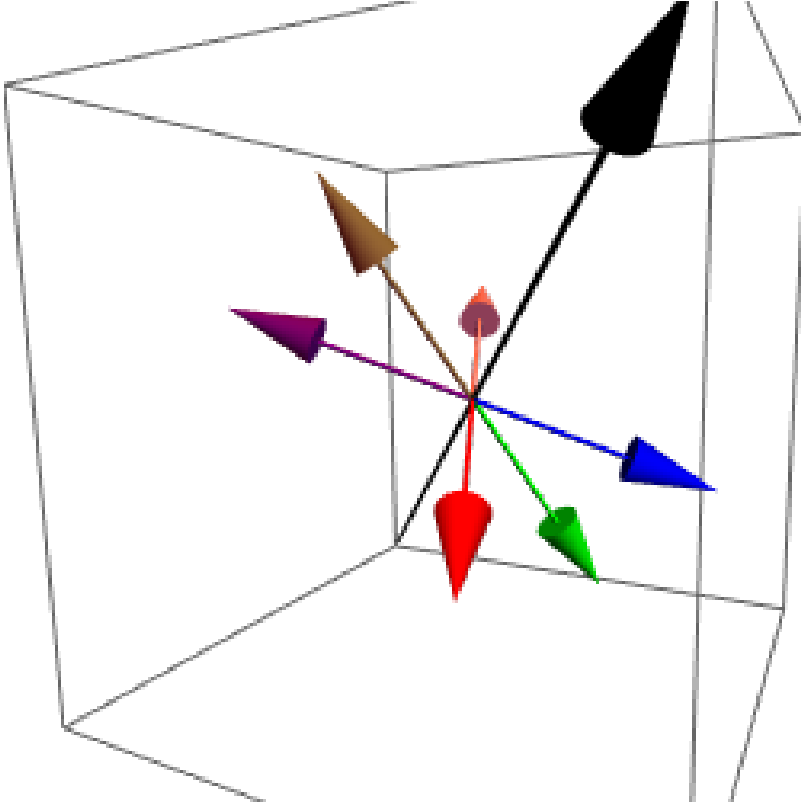


Figure 3.4: The six sublattice spins conjoined at their ends for clarity and illustration. The vector denoting $\langle 1,1,1 \rangle$ axis of symmetry is illustrated in black

By generating the spin vectors described by the equations, spin configurations ranging from planar to non-planar states can be obtained. The following contour plot illustrates the volume of a parallelepiped formed by a spin configuration corresponding to a particular θ and ϕ on the plane of the plot. It is from this illustration that one can obtain an understanding of what choices of θ and ϕ result in planar states or non-planar states.

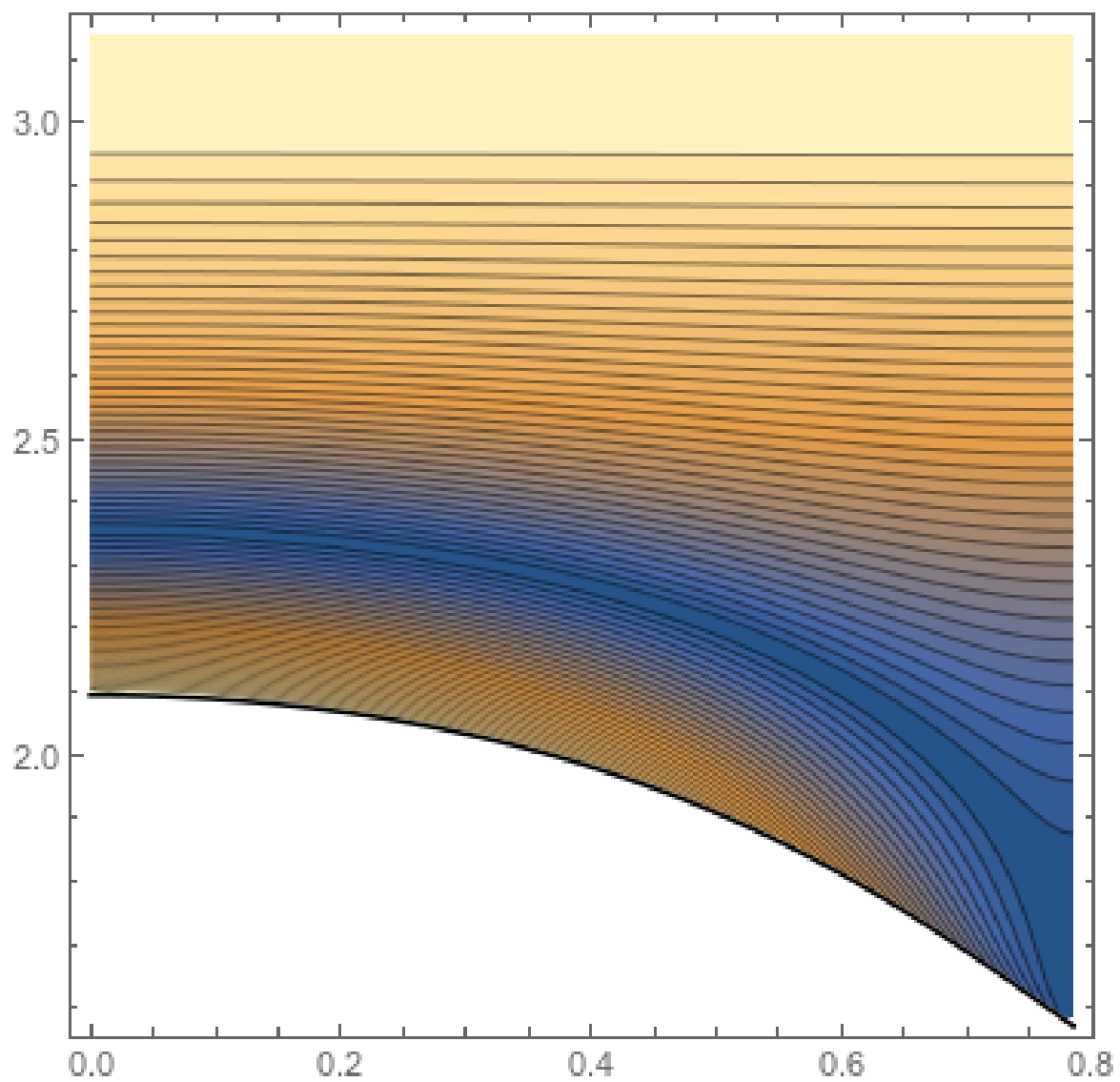
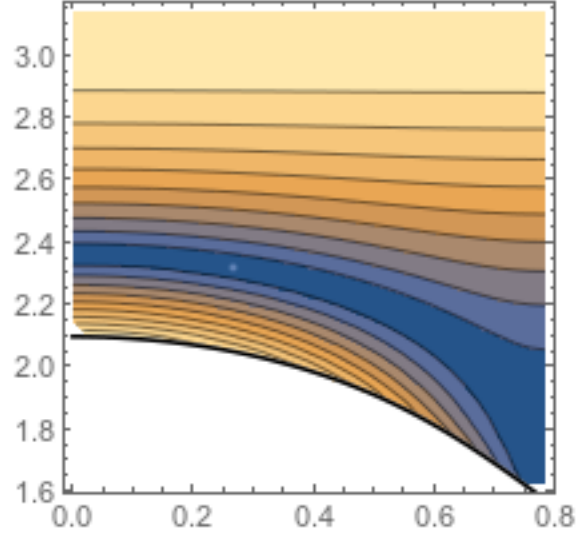


Figure 3.5: A contour plot of volume of a parallelepiped formed by a spin configuration with respect to θ and ϕ



The following plots illustrate some of the possible spin configurations that result from particular choices of θ and ϕ .

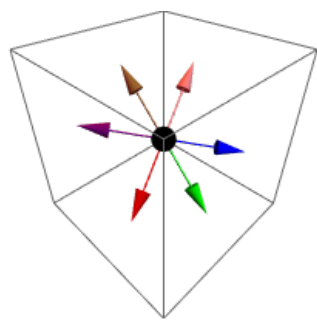


Figure 3.6: View 1

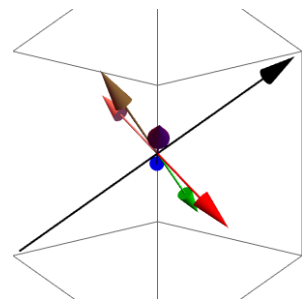


Figure 3.7: View 2

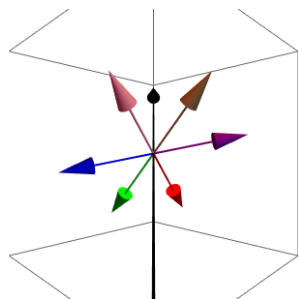


Figure 3.8: View 3

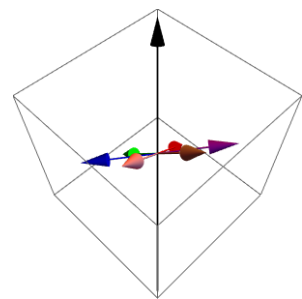


Figure 3.9: View 4

3.1.2 Planar Ground States

The thin strip of blue that cuts into the contour plot just above the complex region consists of the set of points that give rise to parallelopipeds with the smallest volume. This corresponds to spin configurations that are planar. Elsewhere in the plane, the spin configurations are non-planar. The strip of points that give rise to planar states are described by the following polar equations:

$$\phi = \frac{\pi}{4} \cos \gamma \quad (3.6)$$

$$\theta = \frac{\pi}{4} (\sin \gamma + 2) \quad (3.7)$$

The spin configurations that are planar can therefore be described in terms of one parameter, γ , the polar equations which determine θ and ϕ , and the original set of equations.

Appendix A

Extra spectra

A.1 What should go in an appendix?

- raw data, extra images, extra spectra
- manuals or procedures you've written
- code
- detailed explanations of theory that don't fit in your methods chapter
- etc.