ISSN: 2754-4966

Journal of Nanosciences Research & Reports

SCIENTIFIC Research and Community

Research Article

Open Access

# Understanding Magnetic Phase Transitions in Graphene and Finding Ce2Ge2Mg

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**Received:** February 16, 2024; **Accepted:** February 22, 2024; **Published:** March 06, 2024

## Introduction

For 10 weeks, two projects were carried out at the University of Kentucky during the REU research project. The initial project was titled Understanding Magnetic Phase Transitions in Graphene. However, the latter project brought about more abundant results, which involved research based on the discovery of Ce2Ge2Mg crystals.

## Motivation

The main goal during these 10 weeks was to, ultimately, understand magnetic phase transitions in the material, graphene. Graphene is described as a single layer of carbon atoms, laced together in a hexagonal shaped lattice. Graphene has been noted to have magnetic qualities. The second goal was to acquire Ce2Ge2Mg in order to further understand anti-ferromagnetism in quantum spin liquids (QSL'S).

## Research Goals

In order to first understand magnetic phase transitions, I am required to have a knowledge in quantum mechanics. Quantum Mechanics, as a brief explanation, quantum mechanics' main concept is that a small piece of matter (electron, photon, neutron, protons, etc) has both particle and wave-like qualities. These pieces of matter are analyzed in the way they exist and move in our universe. It's a very fundamental part and a cornerstone of Physics. I soon predict I will take the knowledge I acquire regarding quantum mechanics, and apply it to how magnetic phase transitions occur in graphene. I predict I will do so by dealing with the carbon atom, its properties, and how it acts. This will be done, according to my Mentor in this project, Huang Chunli. Later into the program, I also decided to move towards a new project with Gannon, which essentially targets finding Ce2Ge2Mg. Due to the fact that it's more appropriately fitting towards my current skill set, it has potential to be my main project, with the previous project becoming more of a side occupation.

## Research Methods

Literature, lectures, and running laboratory experiments are the methods that I have used for research. In order to understand the project with Chunli, I got to know some basics in quantum mechanics. It is, after all, the essence of this project. I have also been recommended by Chunli to get some background on calculus, linear algebra, complex analysis, vectors, integration, probability, and mathematica. In terms of The crystal project with Gannon, it's important to know the basic principles of Solid State Physics, the book Solid State Physics by Charles Kittel was a key in my understanding of the project. Also, basic information of chemistry and stoichiometry was important, something that is commonly learned in high school chemistry. Below, I will explain the learnings I acquired during the research process over the past 10 weeks.

## Literature Review

The literary sources in tangent to this research project I have acquired and began to read is Richard Feynman's Lectures on Physics Volume Three. My mentor has advised me to start reading the first three chapters, as it covers the fundamentals of quantum physics. The first three chapters go over quantum behavior, which entails experiments with different pieces of matter, the uncertainty principle, and principles of quantum mechanics. Other topics that I documented in the chapters relate to the relation of wave and particle viewpoints and probability amplitudes. Prior to embarking on this project, I had no prior knowledge of Feynman. I trust that he is a credible source for this project, as he is a theoretical physicist, known especially for his work in quantum mechanics. Chapter one of Feynman's work entails the basics of quantum behavior.

Starting with Atomic Mechanics, I have gathered that quantum mechanics, ultimately, describes matter and light behavior on an atomic scale. The main goal of quantum mechanics is to describe how very small objects behave. This was done and demonstrated with the very infamous bullet experiment, where particles behave like bullets. A gun shoots a stream of bullets, which goes through a two holed armor wall to let bullets through, which then meet at a backstop to absorb the bullets when hit. At the backstop, there is a detector for bullets to be stored and accumulated. The main question to be asked was, "What is the probability that a bullet which passes through the holes in the wall will arrive at the backstop at distance x from center?" In order to find the probability, you must find the ratio of bullets that arrive at the detector in a certain time and total number that hit the backstop during that time. A similar experiment was done, this time our material used was electrons. The main conclusion to be drawn was that electrons arrive in lumps like particles, and arrival probability is distributed like wave intensity, so, therefore, it behaves like both a particle and a wave, which is the notion that, in a way, quantum mechanics bases its entire philosophy on. A summary of Quantum Mechanics principles can be tied up in this way:

- The probability of an event in an ideal experiment is given by the absolute square of an absolute value of a complex number, which is referred to as the probability amplitude.
- When an event occurs in alternative ways, the complex number for the event is the sum of the separate waves.
- If an experiment is performed which is capable of determining whether one or another alternative is taken, then P= P1 + P2 (sum of probabilities for each alternative), thus interference is lost.
- The uncertainty principle. Essentially: if you make a measurement on an object, and determine its x component with an uncertainty, you cannot know its x position until it's observed.

The main thing my project with Chunli is centered around is a document entitled "Quartet states in two-electron quantum dots in bilayer graphene", written by Angelika Knothe 1 and Vladimir Fal'ko. To give a quick summary of the article, it basically centers around sing and two particle states of quantum dots in gapped layer graphene (BLG). Ultimately, we want to study short, two-electron, range interactions in graphene, and hopefully that will get us a step closer to relating this phenomenon to magnetism in graphene, which I assume is our main goal. Our focus is not on the whole document, Rather, our main focus is on Appendix G. Where it contains an estimation of short-range couplings. However, we observe that the estimate given at the end of appendix G is wrong. It gives us a negative number, when we want it to be positive. The job given to me and a grad student who has been assisting me, Kyle, is to basically replicate Appendix G. Our starting point is at G10:

$$M = \frac{e^2}{4\pi\epsilon_C\epsilon_0}\int d\mathbf{r}_1^3 \int_{\text{unit cell}} d\mathbf{r}_2^3 \frac{1}{4A|\mathbf{r}_2-\mathbf{r}_1|}\left(u_{K\pm}^{A_1/B_2}\right)^*(\mathbf{r}_1)\left(u_{K\pm}^{A_1/B_2}\right)^*(\mathbf{r}_2)u_{K\pm}^{A_1/B_2}(\mathbf{r}_1)u_{K\pm}^{A_1/B_2}(\mathbf{r}_2)$$

$$\approx \frac{e^2}{4\pi\epsilon_C\epsilon_0}\frac{A}{4}\sum_{\mathbf{R}} e^{i\Delta\mathbf{K}\cdot\mathbf{R}}\iint d\mathbf{r}_1^3 d\mathbf{r}_2^3 \frac{1}{|\mathbf{r}_2-\mathbf{r}_1+\mathbf{R}|}|\varphi_{210}(\mathbf{r}_1)|^2|\varphi_{210}(\mathbf{r}_2)|^2,$$

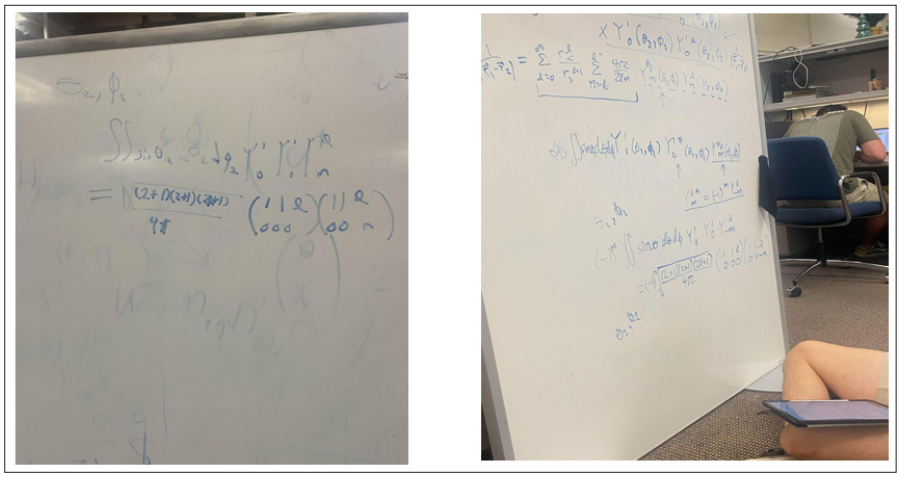
This is referred to as a real space integral. It can be solved in two parts, which in the article, is referred to as R = 0 and R =/= 0. For R = 0, we have the identity

$$\int \sin\theta\, d\theta\, d\phi\, Y_{m_1}^{l_1}(\theta,\phi)Y_{m_2}^{l_2}(\theta,\phi)Y_{m_3}^{l_3}(\theta,\phi) = \sqrt{\frac{(2l_1+1)(2l_2+1)(2l_2+1)}{4\pi}}\begin{pmatrix} l_1 & l_2 & l_3 \\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix} l_1 & l_2 & l_3 \\ m_1 & m_2 & m_3\end{pmatrix},$$

Which then evaluates to:

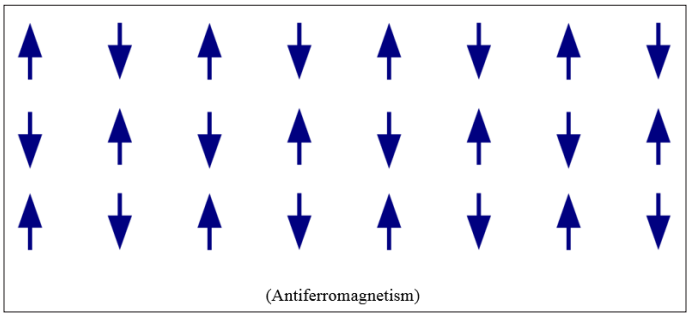
$$\mathcal{M}_0 = \frac{e^2}{4\pi\epsilon_C\epsilon_0}\frac{A}{4}\iint d\mathbf{r}_1^3 d\mathbf{r}_2^3 \frac{1}{|\mathbf{r}_2-\mathbf{r}_1|}|\varphi_{210}(\mathbf{r}_1)|^2|\varphi_{210}(\mathbf{r}_2)|^2 = \frac{e^2}{4\pi\epsilon_C\epsilon_0 a_0}\frac{A}{4}Z\frac{501}{2560}.$$

The project with Chunli has not been so easy for me. Even though I understand the fundamentals I need to know for this project, I have been extremely worried about the kind of outcome I will get when these 10 weeks are over. I feel like even though I know what I need to do, I don't exactly know how to do it. Quantum mechanics is not something a college student fresh out of her second year would exactly be familiar with, and it does not give me much hands-on opportunity. Up until the beginning of the 5th week, where I embarked on a new project with Gannon, much of my time has been spent researching and learning fundamental math and trying my best to read both Feynman and Griffith's books on quantum mechanics. Not only reading them, but understanding them, which is proving to be very difficult for me. However, June 14th, me and Kyle both have gotten started with the R=0 part of the document and calculating it. Turns out there are two parts to the problem: the angular part and the radial part. We figured out the angular part, which evaluates to the following images:



Also, I started to embark on a second project with Gannon, which concerns the material Ce2Ge2MG in crystals. I met with Gannon and he explained to me the background of this project and our main goal. When material is at low temperatures, symmetry is broken, and that results in an antiferromagnetic state, when all neighboring magnetic pulls are anti-parallel to one another. The rest of this technical report will detail this project. During week 5, the radial part of r=0 had been found, thus concluding the first part of reproducing G10 results. I met with Kyle and he showed the calculations he did on mathematica to reproduce the results of the document. I spent week 6 reproducing the mathematica file I was sent.

I then learnt of one of the objectives regarding the crystal project. The main goal is to receive a 2:2:1 atomic percentage ratio of Ce, Ge, and Mg. When looking at our samples collected at the SEM, we, instead, didn't quite receive any success regarding the desired ratios, there was often more Mg than both Ce and Ge, and a huge abundance of carbon in the spectrums. On Thursday, the sample UK 142 was made ready.



(Antiferromagnetism)

**Motivation**

We are looking for the QSL (quantum speed limit) and we want a host, that host being Ce2Ge2Mg. We especially want Mg to act as a flux, but Mg has a lot of entropy behind it, so it hates being a liquid. It wants to go from a solid to the state that has the most entropy: gas. Because of this, it proves very difficult for Mg to act as a flux.

**Flux Method**

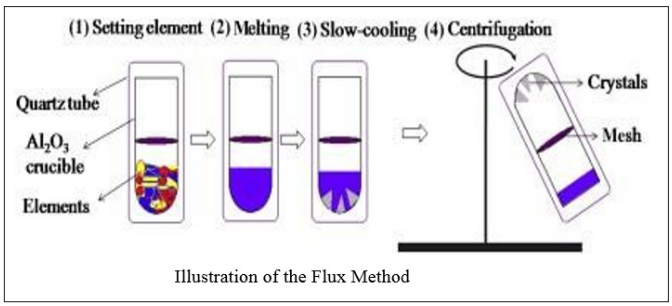
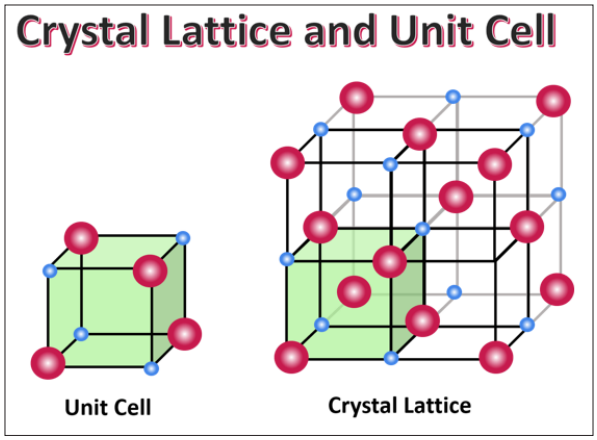



Illustration of the Flux Method

The flux method consists of taking a material, using it as a flux or solvent, putting the materials in a Nb tube due to high vapor pressure of Mg, sealing it in a quartz tube, and putting it in the furnace for an amount of time, with cooling times lasting up to a week in order for crystal formation to occur.

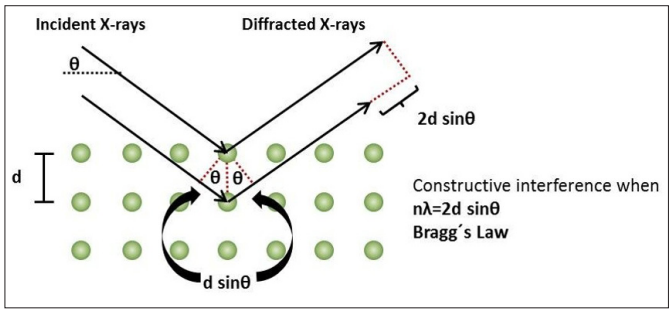
**Solid State Physics and Crystal Structure**

In order to understand Solid State Physics, it begins with beginning to understand the discovery of the X-ray diffraction of crystals and publication of a series of simple crystal calculations, pertaining to its properties and electrons. Kittel explains that crystalline solids hold the most important electronic properties in solids, as properties of important semiconductors are held by crystalline structures, or they are the host. This is reasoned by electrons having extremely short wavelength components that significantly respond to regular periodic atomic order. Crystals formation occurs by the addition of atoms in a constant environment, be it a solution or anything under the correct criteria. This is what is referred to as periodicity. Periodicity is the main property of a crystal. It mainly happens due to the atomic arrangement of the lattice points. As a general statement, crystal structure refers to the repetition of a unit cell.




**X-Ray Significance**

X-rays are waves that have a wavelength that corresponds to the length of the building block of a structure. Kittel states that diffraction proved that crystals are built from a periodic array of atoms. In order to acquire an ideal crystal, they must be built by infinite repetition of atom groups. This grouping is known as the basis. The mathematical points that the basis attaches itself to is referred to as the lattice. We need to know this because of the concept of x-ray diffraction.




**Lattice Properties**

A three-dimensional lattice is made up by three vectors, referred to as a1, a2, and a3. In this way, the atomic arrangement in crystalline solids are identical, regardless if viewed from point r or as from every other point, r', which is translated by integral multiples of a'. The set of points r' for all v-values defines the lattice. A lattice is described as primitive if a unit cell contains only one lattice point, which is made up from the lattice points at each of the corners.

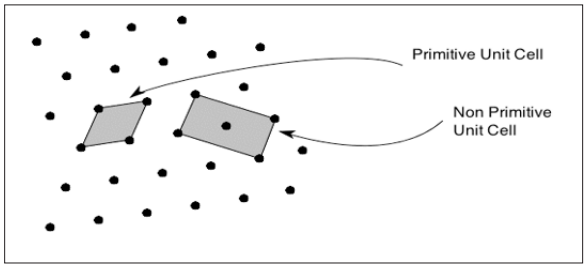
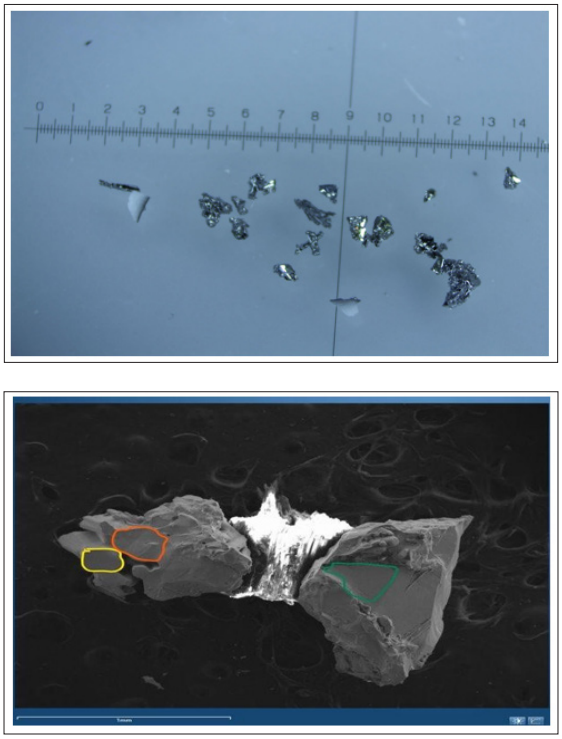
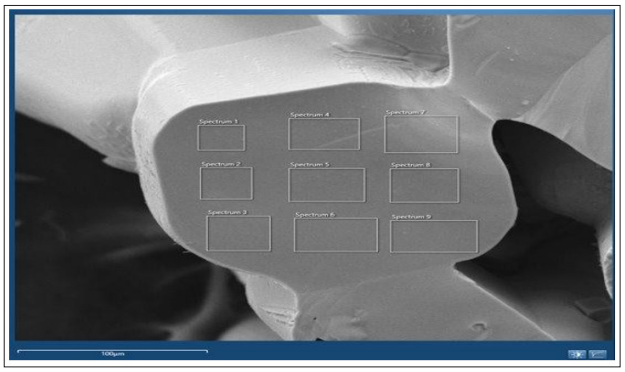



Figure depicting a Primitive Unit Cell and a Non primitive cell, University of Cambridge.



(EDX Image, 2023, Arnold Brennan, UK 144 (left) and UK 145 (right))



(UK 145 Site 1, 2023, Arnold, Brennan)

## Conclusion

Ultimately, we did not acquire a 2:2:1 ratio, but we did find crystal material nonetheless. The next steps for this project would be to simply take our ratios of materials gathered, tweak them, and try again until we can achieve this [1-3].

## References

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3. Angelika Knothe, Vladimir Fal'ko (2020) Quartet states in two-electron quantum dots in bilayer graphene. Physical Review B 101: 235423.