Summary report of GUROP for Sean Boocock (Spring, 2006)

In high school I had a rather idyllic image of physicists. Physicists in my mind sat around brewing over the nature of the universe until they were struck by a revelation at which point they would begin writing down equations on whatever happened to be at hand. It was an image inspired by people like Richard Feynman and Stephen Hawking. Coming to college I was excited by the prospect of working with real physicists and perhaps having an epiphany or two of my own. My experience thus far, particularly this semester, hasn't shattered these notions so much as revealed them for what they were: the fantasies of an outsider looking in at the world of real academic inquiry. Discovering new things, real research, isn't magic and it isn't the emotional roller coaster of a poet caught up in the moment. This semester I have discovered that research can be all the things I had imagined and much more, but not nearly as romantic as I had once conceived it to be.

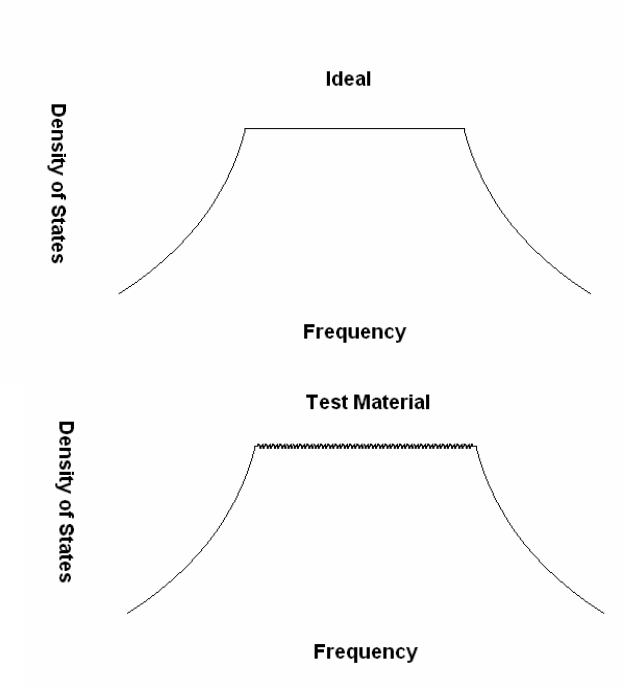
I was motivated to pursue this in part by my experience in Professor Freericks' Relativity and Quantum Mechanics class. While I had a layman's perspective of both subjects, I had never investigated either at depth or even seen the underlying mathematics in the latter case. These mathematics, the wave equations, were very accessible to me at least from a conceptual level. The math also led to several revelations concerning quantum mechanics. One of which was the mathematical reasoning behind the Heisenberg Uncertainty Principle. Working out the mixed operators myself and seeing that one could not measure both velocity and position at the same was very intellectually satisfying. Quantum mechanics spelled the end of scientific determinism and this simple mathematical operation was the final nail in the coffin. At last I understood this principle among others in terms of its mathematical basis.

This was of course only a short and relatively simple introduction to quantum mechanics and its principles. I wanted to explore it more. If physicists have overlooked the difficulties of its interpretation for seventy years because it works so well in practice, I wanted to witness that practice. So I approached Professor Freericks about the possibility of working with him on a project related to his own work in quantum mechanics. At the beginning of the semester, Professor Freericks introduced me to a simple model of the problem I would eventually come to help him visualize. We started with a one dimensional approximation for the motion of electrons. In this model one has evenly spaced lattice sites and electrons are limited to moving from one site to a neighboring site. The question is what is the probability of finding a particle at a specific lattice site for a given energy range. Related to this is the quantity we were after, the density of quantum states. The density of states is a measure of the probability that the electron has a given energy when it is located at a particular lattice site. As energy changes so too does this probability (I thought of it terms of the classical Bohr hydrogen atom – an electron can only occupy a given range of levels for a given energy). After explaining this model, Professor Freericks turned to the ideal 2-d model of the same system. The essential mechanics of this problem are the same but they require a double integral to calculate the density of states. Through substitution one can reduce the system to a one dimensional integral and evaluate the resulting integral as an elliptic integral of the first

kind. I worked out the mathematics of this individually after Professor Freericks' presentation and then graphed the solution as a function of the frequency, or energy, of the particle.

To generate the graph for the 2-d case, I first had to find a program capable of evaluating the elliptic integral. After finding an appropriate C++ program, I modified the program to generate results for different inputs corresponding to the frequency and output the results to a file which I then graphed in excel. The last step was to tackle the ideal 3-d system which was the most relevant to the real world problem Prof. Freericks was investigating. Calculating this integral is significantly more difficult, at least from a coding perspective, in that the integral has limits that vary with a cosine relationship. I am still working on trying to code a program to evaluate the integral correctly.

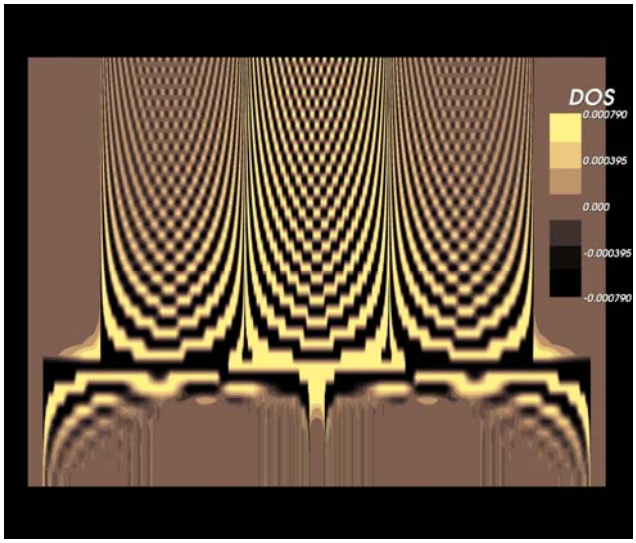
At this point having introduced me to an abstract model of the types of data that he was investigating, Professor Freericks showed me the problem at hand. He was attempting to graph the variation in the density of states of a nanoscale multilayered metal-barrier-metal device. The resistance of the device is related to the density of states at each plane in the device and thus one can determine something of the current flow through the device, given knowledge of its density of states (at least at the atomic level where quantum effects reveal themselves). The structure was split into some 80 planes, 30 metallic, 20 planes of an insulator material, and then 30 more metallic. As one moves through the metal, from one side to the other, the density of states changes subtly. However, trying to visualize these fluctuations, which were akin to ripples in a pond, proved difficult. The ripples are like the superposition of the quantum states of the electrons within the material itself. In the ideal case, as in the figure to the right, these ripples are nonexistent as there are effectively in infinite number of waves superimposed to generate the image. In order to tease out the fluctuations themselves, Professor Freericks thought to subtract the ideal density of states from the calculated value for the material.



This was to be my project, to take the raw data for different planes, subtract the ideal density of states from the raw data, and visualize the results employing an open source, freeware program called Paraview. While a seemingly simple operation, this often proved maddeningly complex in execution. I had just started learning C++ and so the programming tools necessary to perform calculations of this scale were still new to me. I began to tackle the problem by writing several small programs to take the raw data and

strip it of extraneous information, leaving a more formatted data set with which to work. With these new data sets, I then constructed a program to make the necessary subtraction. This proved somewhat difficult as the material is not consistent throughout the 80 planes; the insulator had its own ideal density of states which I initially had to interpolate in order to use with the data sets. For the two months or so that I worked on this project, I rewrote the program I used to make the data correction several times as I learned more advanced concepts in C++ which proved useful. The programming became a project in and of itself for me, and perhaps was the most valuable part of the experience. I was able to apply these new principles that I was learning to a real world problem of some significance which motivated me to code as accurately and elegantly as possible. The final iteration of my program was completely object oriented, utilizing pointers, and containing all the various formatting program/subprograms I had written to make the data presentable.

With the new corrected data, I began the visualization process in Paraview. Paraview, like many open source programs, suffers from an initially unintuitive interface. I first had to spend several hours working through online tutorials in order to get acquainted to the tools and how to manipulate the data to get presentable results. Far more important, and initially harder, was formatting the data to be read by the program. Paraview allows for a wide variety of different data types but they must be formatted according to an open source specification called VTK. Tracking down the specification and implementing it was only the initial challenge. Having formatted the data and done a rudimentary visualization of the data, it was now time to tinker with the settings to produce the best image possible. Since the data had been corrected against the ideal density of states, the resulting residuals were small and the vast majority grouped having a magnitude smaller than 0.002. In order to get the best image, I had to change the color scaling values, use different interpolation options and eventually symmetrize the corrected data after it was discovered that the initial data was not fully symmetric. The final images that I created will be used in a publication.



Throughout this project I was always cognizant of the need for accuracy, which necessitated going back and manually calculating values throughout the data numerous times. This need for careful review was made especially apparent when I discovered, quite by accident, a limitation of C++ that had never been discussed in my programming class. The C++ language only allows for five significant digits in floating point numbers. Trying to work beyond this will result in errors, some of which I encountered while computing the raw data. These and other subtleties were perhaps my greatest revelation

during the semester. The attention to detail in doing a task seemingly as simple as mine made the famous discoveries and theories all the more awe inspiring. I can only imagine the effort that went into the initial formulation of quantum mechanics or Einstein's general theory of relativity. I am not dissuaded though by the difficulty but inspired by the challenge. I found this project to be both rewarding and inspiring and I look forward to continuing it in the future.