

# **ELEC 1908 Assignment 1: Matlab and L<sup>A</sup>T<sub>E</sub>X**

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Due @ 14:25 on Friday February 8th, (Immediately before your lab).

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## Assignment Purpose

A few complex concepts relevant to this degree will be presented, and you will be asked to do a small amount of research and complete a small related task! (This is to provide context and expose you to some very cool concepts in our universe!).

**Purpose 1:** Matlab is an extremely powerful and versatile tool that maintains accessibility due to the comparatively ( $\propto$  to other engineering software tools) shallow learning curve. This assignment will expose you to a few basic uses; plotting, solving equations, producing figures, etc. Feel free to always play with any of the tool kits, and you utilize use Matlab to assist you throughout your degree!

**Purpose 2:** In any degree you will produce a large number of assignments, labs, reports and more. Part of the learning process is being able to consistently produce clear documents to present the ideas and designs you make despite the seemingly vast work load and tight deadlines.  $\LaTeX$  is an incredible word processing tool, use it. Do it, ya won't regret it. It'll be awesome. Utilizing the introduction to Matlab as the material, you will use  $\LaTeX$  for all remaining reports in this course.

## Assignment Outline

### Matlab (50%)

Complete all parts of the **Fermi-Dirac Statistics and Semiconductors** topic below while saving properly labeled and formatted plots for each steps to be included in the final report. Each section will have: X-Y plot, surface plot, and questions to be researched and answered with citations.

### Report Outline and $\LaTeX$ (50%)

What to be included in your final report will be outlined here, please read carefully!

- **Sections:** Introduction (Brief), Table of Contents, Main topic (title related to the question selected, subsections for the research questions), Conclusion (Brief), References, Appendix (containing Matlab code)
- **Plots:** Labeled, referenced in the text (using the  $\LaTeX$  figure referencing command), proper axis labels, overall clear formatting
- **Citations:** IEEE citation style, in text references (Using the  $\LaTeX$ the cite command), reference list at the end
- **Research Questions:** A paragraph or two answering each question for the problem chosen. Must contain references to your research to answer the question, encouraged to use figures and equations to justify your answer.
- **Matlab Plotting Question:** Should have lines of text describing what you're doing and what the problem is. Must include at least one properly formatted equation.

## Topic One: Enrico Fermi

The question requires you to plot the Fermi level function and a surface plot of a constant energy surface.

### Fermi Function Plot

$$f(E) = \frac{1}{1 + e^{(E-E_F)/k_B T}} \quad (1)$$

The Fermi function is a statistically derived description of the chance that electrons (or holes) exist at an energy in an material. Equation 1 is a probability distribution function. This is the most likely arrangement of electrons. This distribution works by describing the probability of occupancy ( $f(E)$ ) as a function of the energy of interest ( $E$ ) at a specific temperature ( $T$ ). Where  $E_F$  is the Fermi level, the 50% occupancy energy level, and  $k_B$  is the Boltzmann constant.

**Plot Equation 1:** for  $T = 300\text{ K}$  and  $E_F = 7\text{ eV}$  across all  $E$ . Label the Fermi level on the plot.

### Constant Energy Surface Plot

Constant Energy solution for simple cubic lattice (SC)

$$\epsilon_k = -\alpha - \gamma(2 \cos(K_x a) + 2 \cos(K_y a) + 2 \cos(K_z a)) \quad (2)$$

If we extend the idea of electrons in a material probabilistically occupying an energy level to the orbitals of the atoms and bonds that make bulk materials. We can start to see how electrons (or holes) move and exist in materials.

A visual giving beautiful insight on materials is the Fermi Constant Energy Surface. As a basic, this is the surface made by tracing a solution (a specific energy occupancy) of the Fermi equation A Fermi surface is a constant energy plot of the valence occupancy of allowed energy states in something called momentum space. The weirdness of Quantum mechanics (QM) can be reduced (infinitesimally) by using two complete set representations to describe reality. The conceptually easy: Time-Space ( $t, x, y, z$ ) (This *should* be familiar, as most people consciously experience time and position [citation needed]), and the abstract: Energy-Momentum ( $E, p_x, p_y, p_z$ ). Using the Energy-Momentum representation of crystal lattice unit cell (a single repeatable unit of a crystalline material) the Fermi Surface encloses the region that electrons can exist within. If it's probabilistic for the occupancy of electrons to exist on the edge of a unit cell a 'bridge' to a neighboring crystal lattice exists and charge can hop along! This charge motion demonstrates conduction within a conduction band permeating a bulk lattice.

**Create a Fermi Surface surface plot** Using a Simple Cubic (SC) crystal lattice (8 atoms arranged in a cube) and working through some math (Using the tight binding approximation for the atoms), it can be found that the energy bands ( $\epsilon_k$ ), is equation 2.

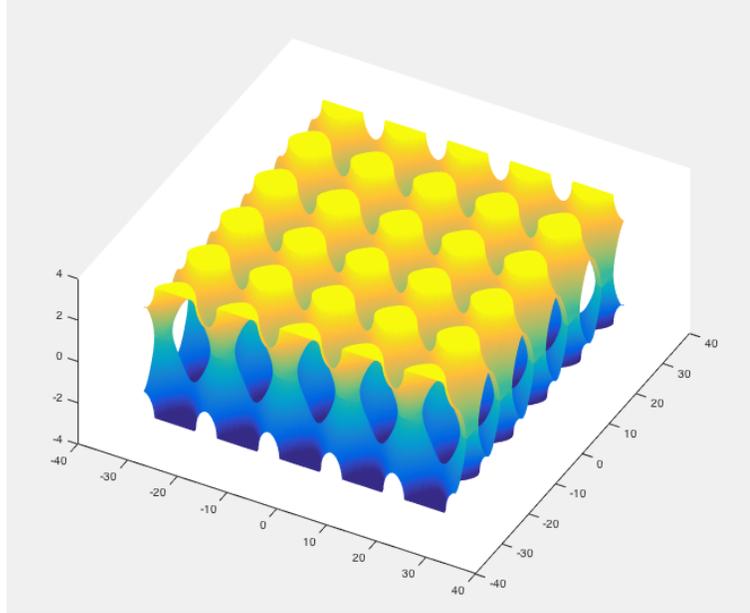


Figure 1: Fermi constant energy surface plot of a SC lattice from across  $5 \times 5 \times 2$  volume of unit cells.

**You will be creating a surface plot, visualizing the regions of high occupancy at a given energy.** To do this, I've substituted some values and rearranged equation 2 into 3. Following the given hints should result in figure 1:

$$z = \cos^{-1}\left(\frac{-(\epsilon_k + \alpha)}{2\gamma} - \cos(0.5x) + \cos(0.5y)\right) \quad (3)$$

- $\alpha = 1.6 \text{ eV}$  and  $\gamma = 3.6046 \text{ eV}$ .
- Create a meshgrid for x and y, from  $6\pi \rightarrow -6\pi$ . (or more, this will just make a bigger and bigger surface)
- Set  $\epsilon_k = \alpha$ .
- Surf(x,y,z). This will create the energy surface for one symmetrical set of atoms that are only horizontally separated.
- Surf(x,y,-z). This will produce the bottom set of atoms.

### Research Questions

Research the following questions and answer them in a paragraph with a minimum of 1 citation each.

- What is the Schrödinger's Equation? What does it describe?
- What is a Semiconductor? Within the context of semiconductors, what is a hole?