NAME _____

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Midterm Exam 1 – PHZ 4404 Spring 2021

SOLID STATE PHYSICS

Thursday, March 4, 2021

Due: Monday, March 8, 2021 at 8 PM at the Canvas site.

This is a take-home exam. It is due on Monday, March 8, 2021 ***at 8 pm (at canvas site).*** You are allowed to use your textbook "Introduction to Solid State Physics" by Kittel and your class notes only (and of course a calculator and a plotting program to do any plots) and you can discuss the questions only with the instructor. You **are not allowed** to work with anyone else. You ***are not*** to use the internet (except for the class pages and any supplemental material on those pages) Your name and signature above indicates that you have obeyed the honor system on this test and have not *received* or *given* aid to or from anyone on this test. There are 105 points on this exam, which includes 5 extra credit/bonus points if you get a perfect score.

Show All Your Work!!!!

- Label all additional work with your name in the upper right hand corner of any additional sheets you turn in.
- All work (on problems) must be shown to receive full credit.
- All work must be **clear** and **unambiguous** to receive full credit. Cross out any work that you do not want counted. If you have the right answer, but wrong steps, you will not receive full credit.
- All units must be shown to receive full credit.
- *Indicate the final answer by **boxing** the result.*

1. **2D Honeycomb Crystal (25 pts).** Graphene, is a two dimensional material (that can be rolled up into "carbon nanotubes") that is an example of a Honeycomb Crystal. (Note that this structure is ***not*** a Bravais lattice.) A honeycomb crystal is shown on the attached page. Let the spacing between adjacent sites be a.

   a. Describe the honeycomb crystal as a Bravais lattice *with a basis*. The underlying 2D Bravais lattice is known as a triangular or hexagonal lattice. Give expressions for the primitive vectors of the Bravais lattice and also the two basis vectors.

   b. Draw the *Wigner-Seitz* cell for this lattice and another, *different* primitive unit cell on the attached sheet.

   c. What is the reciprocal lattice for this honeycomb crystal? Give expressions for the reciprocal lattice primitive vectors.

   d. What is the structure factor, $S_{\mathbf{K}}$, at the reciprocal lattice points **K**?

2. A ***Martensitic Transformation*** **(25 pts).** is a diffusionless transformation**.** According to Wikipedia, "A diffusionless transformation is a phase change that occurs without the long-range diffusion of atoms but rather by some form of cooperative, homogeneous movement of many atoms that results in a change in crystal structure. These movements are small, usually less than the interatomic distances, and the atoms maintain their relative relationships. The ordered movement of large numbers of atoms lead some to refer to these as military transformations in contrast to civilian diffusion-based phase changes."

   Sodium transforms from *bcc* to *hcp* at about 23 K in a ***martensitic transformation***. Assuming the *density* remains constant, find the lattice constant a_{hcp} of the hexagonal phase, given that the *bcc* lattice constant $a_{bcc} = 4.23$ Å (this is the length of the side of the "cube" in the *bcc* lattice and not the nearest neighbor distance) and that the *c/a* ratio for the hexagonal phase is indistinguishable from its ideal value. (You do not need to recalculate the ideal *c/a* ratio, but can use anything in the book etc.)

3. ***1D Cosine Energy Band*** **(25 pts).** Consider a *one dimensional* crystal with lattice constant a and total length L that has an energy band given by $\varepsilon(k) = -\varepsilon_0 \cos(ka)$.
   a. Sketch the energy as a function of k in the first Brillouin zone.
   b. What is the effective mass, m^* at $k = 0$? For k at the Brillouin zone boundary?
   c. What is the maximum electron linear density n (i.e. number/length) for a full band? Assume that two electrons (one spin-up, one spin-down) can go into each allowed state.
   d. For T = 0, find the Fermi energy as a function of linear density n for $n = 0$ to n_{max}.
   e. Calculate the density of states in energy/per unit length $g(\varepsilon)$ for this band and sketch it in the first Brillouin zone.

4. ***Empty Lattice for BCC crystal structure*** **(30 pts).** In this problem, we will plot (with a computer, i.e. not by hand) the empty lattice band structure for a BCC lattice, (i.e. we take the free electron bands and map them back into the first Brillouin zone using reciprocal lattice vectors.) Plot in the [100] direction, the energies of all bands up to five times the lowest band energy at the zone boundary at $\mathbf{k} = (2\pi / a)\,\hat{\mathbf{x}}$ (This is known as the "H" point in the Brillouin zone). You can let this be the unit of energy. This problem shows why band edges need not be at the zone center. Note that the band crossing degeneracies will be removed when one takes into account the crystal potential. **Hint:** It might be useful to make a table like the one on page 176 in your book and follow the results there.

Use for Problem 1: