

Physics 685 – Electronic Structure

Homework 1

Please read Martin, *Electronic Structure*, Chapter 2, particularly sections 1-2, but also 5-6 and 8-9. Come prepared to discuss the following questions based on reading. You not need to answer all of them, nor completely, but you do need to be able to make an effort!

1. What are three properties of a material that are determined by its electronic ground state? Explain each one briefly, including why it requires knowledge of the electronic ground state. What are three properties of a material that require knowledge of electronic excited states?
2. What are the five types of bonds described by the author. Where applicable, what kinds of bands are typical of each? What kinds of crystal structures?
3. How is the electronic density of a covalent bond measured experimentally?
4. Given $E(\Omega)$, the ground state energy as function of volume, and assume it is approximately parabolic with a minimum at Ω_0 .
 - (a) Give a physical interpretation of the bulk modulus B at the minimum. How would B differ between a loosely bound system and a tightly bound system?
 - (b) What must you do to get zero pressure in this system? At what volume does this occur. At what volumes is the pressure positive? negative?
 - (c) How does one find the transition pressure in the plots in, say, Fig. 2.1?
5. What do you think a "frozen phonon" might be? What are you doing to the system in comparison to the ground-state situation? What are you interested in calculating by this technique?
6. Describe the following "allomorphs" of carbon in bulk and at the nanoscale: diamond, graphite, graphene, carbon nanotube, buckyball. Do some wikipedia "research" if need be. What is a potential application of a carbon nanotube?
7. As best you can, describe the difference between the structure of the H defect in p-type and n-type Silicon. What surprising physics did computational simulation reveal in this case? Why do you suppose it would be hard for one to find this out experimentally?