INTRODUCTION TO PART 3

0. Review:
   In working with vibrations in a crystal, we ran into the **quantum theory** in two places.
a) The **wavevectors were quantized** (in the Debye model, $K_\# = \#\pi/L = \#\pi/Na$).   And because the atoms were discrete and not continuous, our max K was limited to π/a with higher K's (K>G) not giving any different oscillation patterns than K's within the Brillouin zone. This limited the number of modes.
b) The **energy** in those waves **was quantized**: $\varepsilon = \hbar\Omega$.   We can have more than one phonon excited for any frequency if we have enough energy, but we can't have fractional phonons.   The probabilities can be fractional, but the actual number has to be an integer.
   The lower frequency waves have a lower energy/phonon and so these phonons have a higher probability to be excited, while the higher frequency waves have a higher energy/phonon but a lower probability to be excited (by the Boltzmann probability distribution).   The Planck distribution gave us the average number of phonons for each mode based on the oscillation frequency and the temperature.
   At high temperatures, the higher phonon energies times the lower probabilities (lower number of phonons) evened out with the lower phonon energies times the higher probabilities (higher number of phonons) to give the same average energy, $k_B T$, per mode – which agreed with the classical theory.

1. Introduction:
   This section is a first look at the **electrical properties** of crystals.   To do this we need to consider the electrons in the crystal.

In **metals**, the outer (valence) electrons can move around in the material so they will contribute to
   (1) the electrical conductivity,
   (2) the thermal conductivity, and since they have energy they can contribute to the internal energy and hence
   (3) heat capacity.
The contributions of the electrons to the second and third properties is **in addition** to the contributions of the oscillations of the atoms in the crystal that we have already considered.

In **insulators**, the electrons cannot move around, so they cannot contribute to the above three cases.

In **semiconductors**, strange things happen.   We will look at what makes them strange in **Part 4** of the course (which will be an extension of what we do in this part).

2. Important considerations:
   We will again need the quantum theory.   The quantum theory explains why there are only certain electrons in an atom (the valence electrons) that are important to the electrical and thermal properties of materials.   In addition:
   2a)   Electrons exhibit the same **wave/particle duality** that photons and phonons do, but the electrons have rest mass, whereas the photons and phonons do NOT.   This means that we will need to use the **Schrodinger's Equation**.
   2b)   Electrons are fermions; that is, electrons are spin ½ particles that obey the **Pauli Exclusion Principle**.   Photons and phonons are bosons that are integer spin particles that are NOT limited by the Pauli Exclusion Principle.   Also, electrons are fixed in number – they cannot be created or absorbed like phonons and photons.   This will lead to a different distribution function, the Fermi-Dirac distribution instead of the Planck distribution.
   (2c)   The valence electrons in metals act as if they were essentially "free" but are in a periodic potential (due to the periodic ion cores).

3. Method of attack:

      (3a) We will first look at **one free electron** (no potential energy).

      (3b) Next we will consider a bunch of free electrons that together are subject to the Pauli Exclusion Principle. We will call this the **free electron Fermi gas**. We will look at the thermal and electrical properties predicted by this model.

      (3c) We will then see what happens when we put in a periodic potential (instead of the "free" electron model). To work with this we will need the Fourier series and the reciprocal lattice vectors (the **G**'s). From this we will get the **energy gap** between energy bands.

In **part 4** we will consider **semiconductors** based on the idea of the energy gap that we get in this part.

Symbols: small k will usually refer to the wavevector of the electron wave: $k = 2\pi/\lambda$, and this k will usually be a vector or a vector component. We will use k_B to refer to Boltzman's constant $= 1.38 \times 10^{-23}$ J/K (J/K = Joules/Kelvin); however, it will not be possible to put the sub B on the k when the k is in the exponent, so when you see something like $e^{-\varepsilon/kT}$, realize that the k in the exponent is Boltzman's constant, not the electron wavevector. Also, since we will mainly be dealing with electrons in Part 3, the symbol, m, will usually stand for the mass of an electron, not the mass of the atom as was the case in Part 2.