Assignment 6

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1 Problem 1 - Kittel 7.1

From Week 7 Slide - 10, we know that the energy of a free electron is given by:

$$E = \frac{\hbar^2 \vec{k}^2}{2m}$$

Where the two-dimensional wave vector $\vec{k}$ is given by:

$$\vec{k} = k_x \hat{i} + k_y \hat{j}$$

For the corner of the first zone: $(k_x, k_y) = (\pi/a, \pi/a)$, which in turn yields an energy of:

$$E_{corner} = \frac{\hbar^2 \pi^2}{ma^2}$$

For the midpoint of a side face of the zone: $(k_x, k_y) = (\pi/a, 0)$, the energy is:

$$E_{side} = \frac{\hbar^2 \pi^2}{2ma^2}$$

This is obviously exactly half of the previous calculation. In a three dimensional system, $\vec{k}$ is given by:

$$\vec{k} = k_x \hat{i} + k_y \hat{j} + k_z \hat{k}$$

And so, for the corner: $(k_x, k_y, k_z) = (\pi/a, \pi/a, \pi/a)$:

$$E_{corner} = \frac{3\hbar^2 \pi^2}{2ma^2}$$

For the side: $(k_x, k_y, k_z) = (\pi/a, 0, 0)$:

$$E_{side} = \frac{\hbar^2 \pi^2}{2ma^2}$$

Again, we see that the corner solution is higher energy by a factor of 3. I think we can conclude that the difference in energy is related to the dimensionality d. I believe that this result is important for divalent metals because of their multiple electrons per unit cell. This energy splitting creates two partially filled bands which provide a finite conductivity to the material.

2 Problem 2 - Kittel 7.3

The Kronig-Penney Model describes the behavior of a free electron in a one-dimensional periodic potential. In order for us to find the energy levels of this system, we must solve the wave equations for the system. The two potential regimes are:

$$V(0 < x < a))_1 = 0$$

$$V(-b < x < 0)_2 = V_0$$

These result in two wave equations (Week 7 Slide 12):

$$\Psi_1(x) = Ae^{ikx} + Be^{-ikx}$$

$$\Psi_2(x) = Ce^{ikx} + De^{-ikx}$$

We can solve for the relevant constants by utilizing boundary conditions. Two of them are continuity at their intersection and the derivative of same (Week 7 Slide 12):

$$\Psi_1(a) = \Psi_2(a)$$

$$\frac{d\Psi_1(a)}{dx} = \frac{d\Psi_2(a)}{dx}$$

If we also do the boundary conditions specified by the Bloch Theorem (and enumerated in full in Week 7 Slides 13-16) results in the following equation:

$$\left[\frac{Q^2 - K^2}{2QK}\right]^2 \sinh Qb \sin Ka + \cosh Qb \cos Ka = \cos k(a+b)$$

As noted on Week 7 Slide 16, if we use a delta function approximation, this equation simplifies to:

$$\frac{P}{Ka}\sin(Ka) + \cos Ka = \cos ka$$

Where:

$$P \equiv \frac{Q^2 ab}{2}$$

If we set $k = 0$ as specified, and examine the $Ka \ll 1$ regime, we simplify to:

$$\frac{P}{Ka}Ka + 1 - \frac{K^2a^2}{2} \simeq 1$$

Which, in turn, gives the following energy (which is also listed in Week 7 Slide - 18):

$$E = \frac{\hbar^2 K^2}{2m}$$

If we instead set $k = \pi/a$, then the equation simplifies to:

$$\left(\frac{P}{Ka}\right)\sin Ka + \cos Ka = -1$$

Again, we have to examine a regime for Ka. Let's toss in a a factor α that is very close to zero: $Ka = \pi + \alpha$. This simplifies the above equation into:

$$\left(\frac{P}{\pi}\right)(-\alpha) - 1 + \frac{\alpha^2}{2} = -1$$

The two solutions to this equation: $\alpha_1 = 0$ and $\alpha_2 = 2P/\pi$ generate an interesting conclusion: a band gap of the following form:

$$E = \frac{\hbar^2\pi^2}{2ma^2} + \frac{\hbar^2\pi\alpha}{ma^2}$$

3 Problem 3

Referring to Cooper et al's article in the 2012 Condensed Matter Physics Journal, 'Experimental Review of Graphene', we learn some interesting things. First:

> Graphene is a zero-gap semiconductor because the conduction and valence bands meet at the Dirac points... The Dirac points are locations in momentum space, on the edge of the Brillouin zone. There are two sets of three Dirac points. Each set is not equivalent with the other set of three. The two sets are labeled K and K' . The two sets of Dirac points give graphene a valley degeneracy of $g_v = 2$. The K and K' points are the primary points of interest when studying the electronic properties of graphene. This is noteworthy in comparison to traditional semiconductors where the primary point of interest is generally Γ, where momentum is zero.

Essentially, the unique two-dimensional structure and symmetry generates unique properties in momentum space that lead to unique electronic band gap features. These features generate some unique electron behavior. Explicitly:

> ...the effective mass of the charge carriers in this region is zero... Charge carriers in graphene behave like relativistic particles with an effective speed of light given by the Fermi velocity. This behavior is one of the most intriguing aspects about graphene and is responsible for much of the research attention that graphene has received

Essentially, graphene's structure makes it extremely good at conduction as long as its crystal structure is pure.