Solid State 1 HW7

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7.1

a) The energy of a free electron gas in two and three dimensions is:

$$E_{2D} = \frac{\hbar^2}{2m}\left(k_x^2 + k_y^2\right) \tag{0.1}$$

$$E_{3D} = \frac{\hbar^2}{2m}\left(k_x^2 + k_y^2 + k_z^2\right) \tag{0.2}$$

The corner point at $k_y = k_x = \pi/a$ then has twice the energy of the k vector halfway along the side at $k_x = \pi/a, k_y = 0$.
b) The corner point at $k_z = k_y = k_x = \pi/a$ has three times the energy of the k vector halfway along the side at $k_x = \pi/a, k_z = k_y = 0$.
c)

7.3

a) The Kronig-Penney model is:

$$(P/Ka)\sin Ka + \cos Ka = \cos ka \tag{0.3}$$

We are looking for the lowest energy band when $k = 0$ with $P \ll 1$. Assuming the first term is small due to the condition on P, and noting that $\underline{\lim}_{x\to 0} \sin x/x = 1$, we have:

$$K \simeq 0, k = 0 \tag{0.4}$$

$$\cos Ka \simeq 1 - P \tag{0.5}$$

$$K \simeq \frac{1}{a}\cos^{-1}(1-P) \tag{0.6}$$

The energy of the lowest band at $k = 0$ is $\frac{\hbar^2}{2ma^2}\left(\cos^{-1}(1-P)\right)^2$.
b) At $k = \pi/a$ we have:

$$\frac{P}{Ka}\sin Ka + \cos Ka = -1 \tag{0.7}$$

To find the band gap we need to find the points at which the function is equal to -1. We note that the sinc function $\sin x/x$ has zeros at $x = \pm n\pi$ with n an integer, so one of the points is at $Ka = \pi$. Expaning both the sinc function and $\cos x$ about $x = \pi$ we have:

$$P(1 - x/\pi) - 1 + \frac{1}{2}(x - \pi)^2 = -1 \tag{0.8}$$

$$P(1 - x/\pi) + \frac{1}{2}(x - \pi)^2 = 0 \tag{0.9}$$

We don't find a closed-form expression from this, but plugging in $P = 0.1$ we find the second solution at $x = 3.205, K = 3.205/a$. This gives a band gap of $\frac{\hbar^2}{2ma^2}(3.205^2 - \pi^2)$.

Q3

Examining the band structure of graphene in figure 2 of Electron and Phonon Properties of Graphene we see that the top valence band (π) and the conduction band ($\pi*$) meet at the K point. This crossing of the valence and conduction bands at a specific point explains the high conductivity of graphene.