Solid State Physics
Exercise Sheet 9
Electronic band structure

HS19
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Exercise 1 *Kronig-Penney Model*

With this exercise, we will solve the Kronig-Penney model in small steps. This model starts with the assumption that the potential that the electron feels near the atomic positions can be approximated by a δ-function. The periodic potential can thus be written as $U(x) = Aa\sum_s \delta(x - sa)$ (in one dimension) where A is a constant and a is the lattice spacing.

(a) Show that in the Fourier series $U(x) = \sum_G U_G e^{iGx}$ we get for the coefficients $U_G = A$.

(b) Let $\psi(k)$ be the Fourier coefficients of the electron wave function. Use the central equation (derived in the lecture or found in text books and on the web) to show that

$$(\lambda_k - \epsilon)\psi(k) + A\sum_n \psi(k - 2\pi n/a) = 0 \tag{1}$$

where $\lambda_k = \hbar^2 k^2/2m$.

(c) Now we are interested in solving with respect to ϵ. In this context it is convenient to define $f(k) = \sum_n \psi(k - 2\pi n/a)$. Show that (Caution: n has two meanings):

$$\psi(k) = -\frac{(2mA/\hbar^2)f(k)}{k^2 - (2m\epsilon/\hbar^2)} \tag{2}$$

$$f(k) = f(k - 2\pi n/a) \tag{3}$$

$$\psi(k - 2\pi n/a) = -\frac{(2mA/\hbar^2)f(k)}{(k - 2\pi n/a)^2 - (2m\epsilon/\hbar^2)} \tag{4}$$

(d) Now let's sum ($\sum_n$) on both sides of equation 4 found above and show that:

$$\hbar^2/2mA = -\sum_n \left[(k - 2\pi n/a)^2 - (2m\epsilon/\hbar^2)\right]^{-1} \tag{5}$$

Notice how with these simple operations we got rid of the Fourier coefficients of the wave function ψ.

(e) Our goal is still to solve with respect to ϵ. Let's define $K^2 = 2m\epsilon/\hbar^2$ and remember that $\cot(x) = \sum_n \frac{1}{n\pi + x}$. Show that:

$$\frac{\hbar^2}{2mA} = \frac{a^2\sin(Ka)}{2Ka(\cos(ka) - \cos(Ka))} \tag{6}$$

Hint: It is helpful to use a partial fraction decomposition of equation 5. The following trigonometric identities might be useful:

$$\cot x - \cot y = \frac{\sin(y - x)}{\sin x \sin y} \tag{7}$$

$$2\sin x \sin y = \cos(x - y) - \cos(x + y) \tag{8}$$

(f) What is the energy of the lowest energy band at $k = 0$ if we assume $P = \frac{mAa^2}{\hbar^2} \ll 1$? (Hint: how big can Ka be? If it is small, you can expand in Ka.)

(g) Evaluate the band gap at the zone boundary $k = \pi/a$ (we still assume $P \ll 1$).

(h) Now let us set $P = 3\pi/2$. Plot the dispersion relation from 0 to $4\pi/a$. Plot also the same dispersion in the reduced zone scheme (all bands folded into first zone). Use a computer for the plots! (Hint: You have to solve equation 6 numerically. If you do not see any energy gaps, you did something wrong. Furthermore, the dispersion relation should look somewhat parabolic. Pay attention to the starting values.)