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Due on 11th May

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

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

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):

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

$$f(k) = f(k - 2\pi n/a) \quad (3)$$

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

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

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

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:

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

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

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

$$2 \sin x \sin y = \cos(x-y) - \cos(x+y) \quad (8)$$

- (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.)