BAND STRUCTURE OF SOLIDS: DEGENERACY OF STATES

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

References: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 5.21.

In the band-gap model of one-dimensional solids, each band covers a range of energies such that

$$\cos\theta a = \cos z + \beta\frac{\sin z}{z} \tag{0.1}$$

has valid values for the cosine on the LHS (where $\theta = \frac{2\pi n}{Na}$, with N being the number of atoms in the loop and a the spacing of the delta function spikes). The variable z (which depends ultimately on the energy) varies over values making the RHS lie in the range $[-1,1]$. Within one band, $\theta a = 2\pi n/N$ thus varies between 0 and π.

Since $\cos x = \cos(2\pi - x)$, $\cos\theta a$ has the same values for $\theta a = 2\pi n/N$ and $\theta a = 2\pi(N-n)/N$ so these two states have the same energy. The only exceptions are firstly, $n = 0$ (since the maximum value of n is $N-1$, there is only one state with $\cos\theta a = +1$) and secondly, $n = N/2$ (which gives $\cos\theta a = -1$, but exists only if N is even). Thus energies at the top and bottom (or top only, for N odd) are non-degenerate.