

BAND STRUCTURE OF SOLIDS: DEGENERACY OF STATES

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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

$$(1) \quad \cos \theta a = \cos z + \beta \frac{\sin z}{z}$$

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.