BAND STRUCTURE OF SOLIDS: NUMERICAL SOLUTION

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References: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 5.19.

In the band-gap model of one-dimensional solids, the potential is a periodic sequence of delta functions with a spacing of a:

$$V(x)=\alpha\sum_{j=1}^{N-1}\delta(x-ja) \tag{1}$$

By imposing boundary conditions and using Bloch's theorem, we arrived at the relation

$$\cos(\theta a)=\frac{m\alpha}{\hbar^{2}k}\sin(ka)+\cos(ka) \tag{2}$$

where

$$\theta = \frac{2\pi n}{Na} \tag{3}$$

$$k^{2} = \frac{2mE}{\hbar^{2}} \tag{4}$$

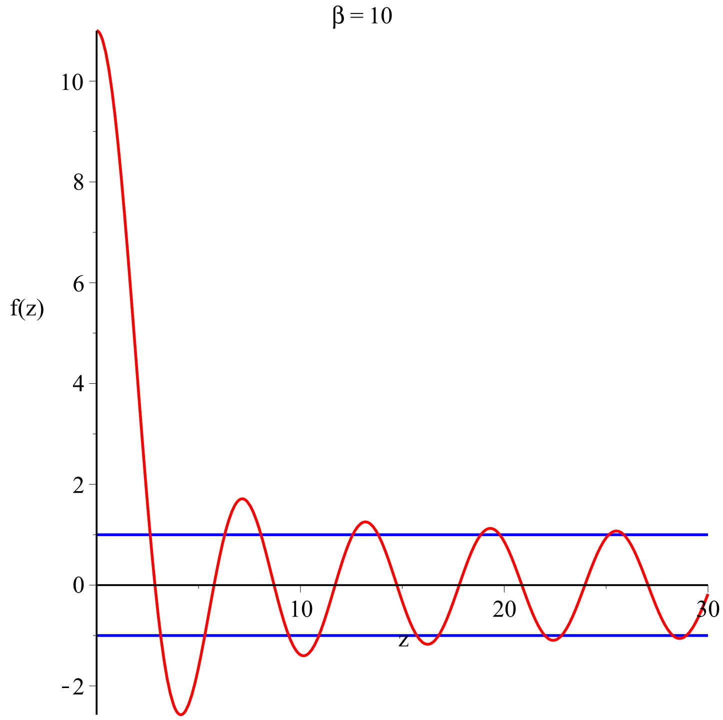
If we define $z\equiv ka$ and $\beta\equiv m\alpha a/\hbar^{2}$ then the RHS of this is a function of z:

$$\frac{m\alpha}{\hbar^{2}k}\sin(ka)+\cos(ka)=\beta\frac{\sin z}{z}+\cos z\equiv f(z) \tag{5}$$

By requiring $\cos(\theta a)\le 1$, we find that $z=ka$ is restricted to certain ranges or bands, which means that electron states are restricted to the corresponding energy ranges. We can find the boundaries of these bands by looking for the values of z at which $f(z)=\pm 1$.

Although in the general case we'll need to solve this equation numerically, we can actually get half the solutions right away by noticing that whenever $ka=j\pi$ for some integer j, $f(z)=(-1)^{j}$. Thus half the boundaries will be at multiples of π. There is no simple formula for finding the other half, though.

As a reminder of what we're trying to solve, the points we're looking for are those where the red curve intersects the blue lines:



We can use Maple's fsolve command to find numerical solutions. After defining $f(z)$ in Maple, we can find the bottom of the first band with the command fsolve(f(z)=1,z=2..3). This gives a value of $z = 2.627675$ if $\beta = 10$. To convert this to an energy, we have

$$E = \frac{\hbar^2 (ka)^2}{2ma^2} \tag{6}$$

$$= \frac{\alpha z^2}{2a\beta} \tag{7}$$

To get a value, we need to know α/a, so if we arbitrarily specify this to be 1 eV, then E for the bottom of the band is

$$E = \frac{(2.627675)^2}{20} = 0.345 \text{ eV} \tag{8}$$

The top of the lowest band is at $z = \pi$ giving $E = 0.493$ eV.