

BAND STRUCTURE OF SOLIDS: NEGATIVE ENERGIES

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References: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 5.20.

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

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

A slightly more realistic potential might be a sequence of delta function wells rather than spikes, since the electron feels an attraction to each of the nuclei. That is, we can instead take

$$V(x) = -\alpha \sum_{j=1}^{N-1} \delta(x - ja) \quad (2)$$

where $\alpha > 0$ is the strength of each well. You might think that this requires only changing the sign of α in the solution we got for delta function spikes, but because the potential now has negative portions, there will be negative energy solutions as well. Fortunately, we've already worked out the method for the solution.

For the region $0 < x < a$, the solution is

$$\psi(x) = Ae^{-\kappa x} + Be^{\kappa x} \quad (3)$$

where $\kappa = \sqrt{-2mE}/\hbar$ (with $E < 0$).

Because the potential is periodic, we can use Bloch's theorem to get the solution for $-a < x < 0$:

$$\psi(x) = e^{-i\theta a} \left(Ae^{-\kappa(x+a)} + Be^{\kappa(x+a)} \right) \quad (4)$$

where $\theta = \frac{2\pi n}{Na}$, with N being the number of atoms in the loop.

Continuity at $x = 0$ gives

$$A + B = e^{-i\theta a} \left(Ae^{-\kappa a} + Be^{\kappa a} \right) \quad (5)$$

The derivatives on either side of $x = 0$ are

$$\psi'_+ = \kappa(B - A) \quad (6)$$

$$\psi'_- = \kappa e^{-i\theta a} (B e^{\kappa a} - A e^{-\kappa a}) \quad (7)$$

From the condition

$$-\frac{\hbar^2}{2m} \Delta \psi' = \alpha \psi(0) \quad (8)$$

we get, using 5

$$\kappa(B - A) - \kappa e^{-i\theta a} (B e^{\kappa a} - A e^{-\kappa a}) = -\frac{2m\alpha}{\hbar^2} (A + B) \quad (9)$$

$$\kappa(B - A) - \kappa(A + B) + 2A\kappa e^{-i\theta a} e^{-\kappa a} = -\frac{2m\alpha}{\hbar^2} (A + B) \quad (10)$$

$$A \left[-\kappa + \kappa e^{-i\theta a} e^{-\kappa a} + \frac{m\alpha}{\hbar^2} \right] = -\frac{m\alpha}{\hbar^2} B \quad (11)$$

$$A \left[\frac{\kappa \hbar^2}{m\alpha} (1 - e^{-i\theta a} e^{-\kappa a}) - 1 \right] = B \quad (12)$$

Substituting back into 5 we get

$$\frac{\kappa \hbar^2}{m\alpha} (1 - e^{-i\theta a} e^{-\kappa a}) = e^{-i\theta a} \left[e^{-\kappa a} + \frac{\kappa \hbar^2}{m\alpha} (e^{\kappa a} - e^{-i\theta a}) - e^{\kappa a} \right] \quad (13)$$

$$\frac{\kappa \hbar^2}{m\alpha} (e^{i\theta a} - e^{-\kappa a}) = e^{-\kappa a} + \frac{\kappa \hbar^2}{m\alpha} (e^{\kappa a} - e^{-i\theta a}) - e^{\kappa a} \quad (14)$$

$$\frac{\kappa \hbar^2}{m\alpha} (e^{i\theta a} + e^{-i\theta a} - e^{\kappa a} - e^{-\kappa a}) = e^{-\kappa a} - e^{\kappa a} \quad (15)$$

$$\frac{\kappa \hbar^2}{m\alpha} (\cos \theta a - \cosh \kappa a) = -\sinh \kappa a \quad (16)$$

$$\cos \theta a = \cosh \kappa a - \frac{m\alpha}{\kappa \hbar^2} \sinh \kappa a \quad (17)$$

Defining $z \equiv \kappa a$ and $\beta \equiv m\alpha a / \hbar^2$ we get

$$\cos \theta a = \cosh z - \beta \frac{\sinh z}{z} \equiv f_-(z) \quad (18)$$

The positive energy solutions are the same as we worked out earlier, with the sign of α changed:

$$\cos \theta a = \cos z - \beta \frac{\sin z}{z} \equiv f_+(z) \quad (19)$$

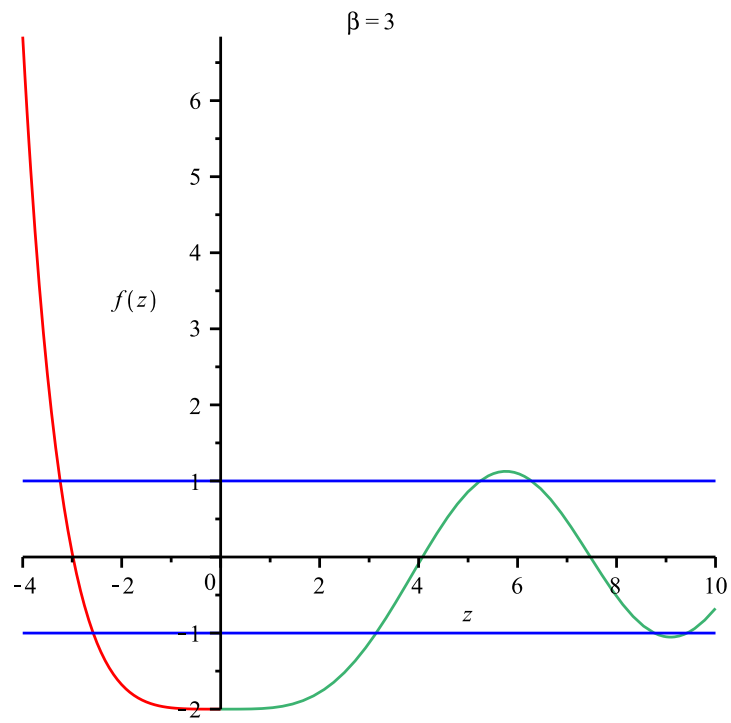
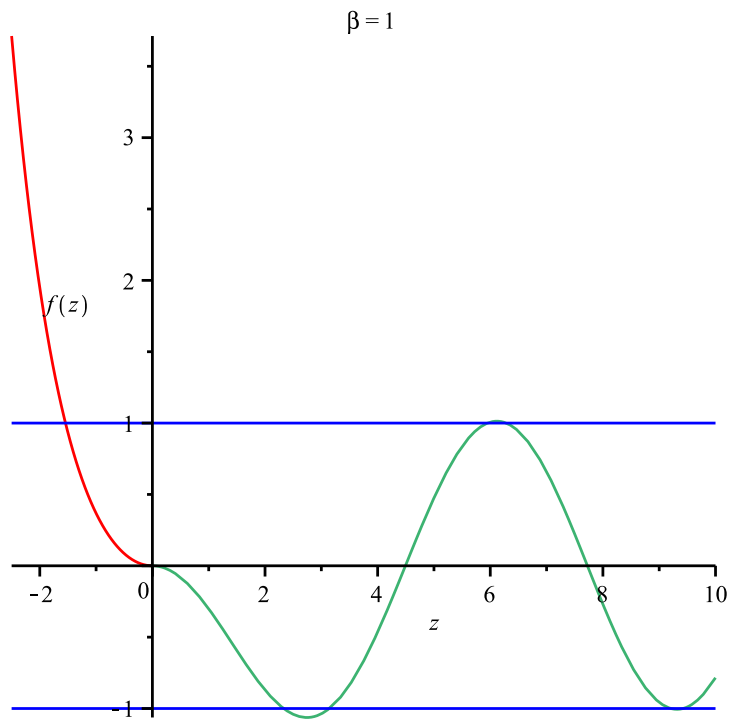
In his question, Griffiths says that the plot showing the band structure must now extend into negative z territory. As far as I can tell, this is just a device that allows the positive and negative energy bands to be displayed on the same plot. Since $z = \kappa a$ and the energy is $E = -\hbar^2 \kappa^2 / 2m$ it is only the square of κ that has physical significance, so we could define it as $\kappa = \pm \sqrt{-2mE} / \hbar$. Therefore, we define $f_-(z)$ only for $z \leq 0$ and $f_+(z)$ only for $z \geq 0$.

The negative energy band can be a separate band, or it can merge with the lowest positive energy band, depending on β . In order for the two bands to merge, the positive and negative solutions must meet at $z = 0$ with a value between -1 and 1 . Because $\lim_{z \rightarrow 0} \sinh z / z = \lim_{z \rightarrow 0} \sin z / z = 1$ and $\cosh 0 = \cos 0 = 1$, $f_+(0) = f_-(0)$ for all values of β , but to satisfy the constraint, we need

$$-1 < 1 - \beta < 1 \quad (20)$$

$$0 < \beta < 2 \quad (21)$$

The plots for a couple of values of β are:



The red curve is $f_-(z)$ and the green curve is $f_+(z)$ with the blue lines showing acceptable solution range. For $\beta = 1$ the negative and lowest positive bands merge, while for $\beta = 3$, the negative energy band is separate.

Since $\theta = \frac{2\pi n}{Na}$ all bands contain $\frac{N}{2}$ energy levels, since $\cos\theta a$ ranges between -1 and 1 . This makes a total of N electron states in each band because of the two spin states at each energy level. In the $\beta = 1$ case, the lowest band splits its N states equally between positive and negative energies, while for $\beta = 3$ the lowest band contains N negative energy states and all higher bands contain N positive energy states.