Solutions
Chapter 7

Problem 3

Part a

We start with equation 21b of the textbook:

$$(P/Ka)\sin(Ka) + \cos(Ka) = \cos(ka). \tag{1}$$

For $k = 0$,

$$(P/Ka)\sin(Ka) + \cos(Ka) = 1. \tag{2}$$

Then, as $P \to 0$, $Ka \to 0$. Hence, for $P \ll 1$, $Ka \ll 1$. So, in this approximation, keeping up to square terms in Ka in the series expansion of sine and cosine, we get,

$$P + 1 - \frac{(Ka)^2}{2} = 1. \tag{3}$$

This gives,

$$K^2 = \frac{2P}{a^2}. \tag{4}$$

Equation 13 of the textbook gives

$$\epsilon = \frac{\hbar^2 K^2}{2m}. \tag{5}$$

So, for the K^2 found above, we get the energy to be,

$$\epsilon = \frac{\hbar^2 K^2}{2m} = \frac{\hbar^2 P}{ma^2}. \tag{6}$$

Part b

Using equation 1 above, the lower edge of the band gap can be seen to be at $ka = Ka = \pi$. Hence, the energy of the lower edge is given by equation 5 to be

$$\epsilon_b = \frac{\hbar^2 \pi^2}{2ma^2}. \tag{7}$$

For $P \ll 1$, the Ka for the upper edge is expected to be larger than π by only a small amount. Hence, we choose

$$Ka = \pi + \alpha, \quad \alpha \ll 1. \tag{8}$$

Then equation 1 gives

$$\frac{P\sin(\pi + \alpha)}{\pi + \alpha} + \cos(\pi + \alpha) = -1. \tag{9}$$

This leads to

$$-\frac{P\sin(\alpha)}{\pi+\alpha}-\cos(\alpha)=-1. \tag{10}$$

Then expanding the sine and cosine in powers of α and keeping up to square terms gives

$$-\frac{P\alpha}{\pi+\alpha}-1+\alpha^2/2=-1. \tag{11}$$

As $\alpha \neq 0$, we get

$$\alpha(\pi+\alpha)=2P. \tag{12}$$

As $\alpha \ll 1$, the relevant root of this equation is

$$\alpha=-\pi/2+\frac{\pi}{2}\left(1+\frac{8P}{\pi^2}\right)^{1/2}. \tag{13}$$

Expanding the quantity in parentheses in powers of P and keeping up to the linear term gives

$$\alpha=2P/\pi. \tag{14}$$

So, for the upper edge of the band gap,

$$Ka=\pi+2P/\pi. \tag{15}$$

Using this in equation 5 gives the energy of the upper edge to be

$$\epsilon_t=\frac{\hbar^2(\pi+2P/\pi)^2}{2ma^2}. \tag{16}$$

Once again for $P \ll 1$, this approximates to

$$\epsilon_t=\frac{\hbar^2(\pi^2+4P)}{2ma^2}. \tag{17}$$

Hence, energy gap is

$$\epsilon_g=\epsilon_t-\epsilon_b=\frac{\hbar^2(\pi^2+4P)}{2ma^2}-\frac{\hbar^2\pi^2}{2ma^2}=\frac{2\hbar^2P}{ma^2}. \tag{18}$$