HOMEWORK 9 SOLUTIONS

36) $$\psi = e^{ikx} A\left(1+be^{-2\pi i x/a}\right) = A\left[e^{ikx} + b e^{-i\left(\frac{2\pi}{a}-k\right)x}\right]$$

$$\psi' = A\left[ike^{ikx} - i\left(\frac{2\pi}{a}-k\right)be^{-i\left(\frac{2\pi}{a}-k\right)x}\right]$$

$$\psi'' = A\left[-k^2e^{ikx} - \left(\frac{2\pi}{a}-k\right)^2 be^{-i\left(\frac{2\pi}{a}-k\right)x}\right]$$

Write
$$V = V_0 \cos\frac{2\pi}{a}x = \frac{V_0}{2}\left[e^{2\pi i x/a} + e^{-2\pi i x/a}\right]$$

$$H\psi = -\frac{\hbar^2}{2m}\cancel{A}\left[-k^2e^{ikx} - \left(\frac{2\pi}{a}-k\right)^2 be^{-i\left(\frac{2\pi}{a}-k\right)x}\right]$$

$$+\frac{V_0}{2}\left[e^{2\pi i x/a} + e^{-2\pi i x/a}\right]\cancel{A}\left[e^{ikx} + be^{-i\left(\frac{2\pi}{a}-k\right)x}\right]$$

$$= E\cancel{A}\left[e^{ikx} + be^{-i\left(\frac{2\pi}{a}-k\right)x}\right]$$

As we do the $V\psi$ multiplication there will be terms to discard:

$$V\psi = \frac{V_0}{2}A\left[e^{i\left(\frac{2\pi}{a}+k\right)x} + e^{-i\left(\frac{2\pi}{a}-k\right)x} + be^{ikx} + be^{-i\left(\frac{4\pi}{a}-k\right)x}\right]$$

$$\text{as } k\to \pi/a \qquad \downarrow \underbrace{e^{3\pi i x/a}}_{\text{discard}} \qquad \downarrow e^{-i\pi x/a} \qquad \downarrow e^{i\pi x/a} \qquad \downarrow \underbrace{e^{-3\pi i x/a}}_{\text{discard}}$$

This leaves.

$$\frac{\hbar^2k^2}{2m}e^{ikx} + \frac{\hbar^2}{2m}\left(\frac{2\pi}{a}-k\right)^2 be^{-i\left(\frac{2\pi}{a}-k\right)x} + \frac{V_0}{2}e^{-i\left(\frac{2\pi}{a}-k\right)x}$$

$$+\frac{V_0}{2}be^{ikx} = Ee^{ikx} + Ebe^{-i\left(\frac{2\pi}{a}-k\right)x}$$

Pick off the coefficients that multiply e^{ikx} and $e^{-i\left(\frac{2\pi}{a}-k\right)x}$

to get $\boxed{\frac{\hbar^2k^2}{2m} + \frac{V_0}{2}b = E}$ and $\boxed{\frac{\hbar^2}{2m}\left(\frac{2\pi}{a}-k\right)^2 b + \frac{V_0}{2} = E\cdot b}$

I will first solve for b. Eliminating E gives

$$\frac{\hbar^2}{2m}\left(\frac{2\pi}{a}-k\right)^2 b + \frac{V_0}{2} = \frac{\hbar^2}{2m}k^2 b + \frac{V_0}{2}b^2$$

Now write

$$k = \frac{\pi}{a} + \delta$$

where we want δ positive (negative) for k just above (below) π/a.

Then
$$\frac{\hbar^2}{2m}\left(\frac{\pi}{a}-\delta\right)^2 b + \frac{V_0}{2} = \frac{\hbar^2}{2m}\left(\frac{\pi}{a}+\delta\right)^2 b + \frac{V_0}{2}b^2$$

$$+\frac{\hbar^2}{2m}\left[\cancel{\left(\frac{\pi}{a}\right)^2} - 2\delta\frac{\pi}{a} + \cancel{\delta^2}\right]b + \frac{V_0}{2} = \frac{\hbar^2}{2m}\left[\cancel{\left(\frac{\pi}{a}\right)^2} + 2\delta\frac{\pi}{a} + \cancel{\delta^2}\right]b + \frac{V_0}{2}b^2$$

$$V_0 b^2 + 8\frac{\hbar^2}{2m}\frac{\pi}{a}\delta\, b - V_0 = 0$$

With

$$\alpha \equiv 4\frac{\hbar^2}{2m}\frac{\pi}{a}\delta$$

we have

$$b = \frac{-\alpha \pm \left[\alpha^2 + V_0^2\right]^{\frac{1}{2}}}{V_0}$$

The trick now is to pick the correct root. We want the one that lets $b \to 0$ as $V_0 \to 0$ which means the $+$ sign for α positive (k above π/a) and the $-$ sign for α negative (k below π/a).

$$b_{above} = \frac{-\alpha + \left[\alpha^2 + V_0^2\right]^{\frac{1}{2}}}{V_0} \qquad b_{below} = \frac{-\alpha - \left[\alpha^2 + V_0^2\right]^{\frac{1}{2}}}{V_0}$$

Now we can let δ go to zero $\Rightarrow$ $\alpha \to 0$ $\Rightarrow$

$$b = \begin{cases} +1 & k \to \pi/a \text{ from above} \\ -1 & k \to \pi/a \text{ " below} \end{cases}$$

$$E = \frac{\hbar^2 k^2}{2m} + \frac{V_0}{2}b \quad \Rightarrow$$

So

$$E = \begin{cases} \dfrac{\hbar^2 k^2}{2m} + \dfrac{V_0}{2} & k \to \frac{\pi}{a} \text{ from above} \\ \dfrac{\hbar^2 k^2}{2m} - \dfrac{V_0}{2} & k \to \frac{\pi}{a} \text{ " below} \end{cases}$$

and the discontinuity is $\boxed{\Delta E = V_0}$

37) (a) We need to do this numerically. Look for values of αa that give $\cos\alpha a - P\sin\alpha a/\alpha a = \pm 1$. For the 1st gap we want αa a bit under π and the function should be -1. Given αa, the energy is given by

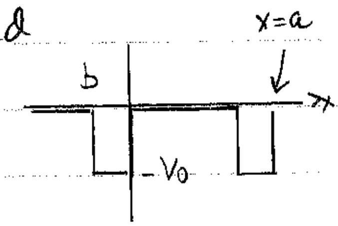
$$E = \frac{\hbar^2\alpha^2}{2m} = \frac{\hbar^2(\alpha a)^2}{2ma^2} = \frac{\pi^2\hbar^2}{2ma^2}\left(\frac{\alpha a}{\pi}\right)^2$$

The gap is from the αa value found above to $\alpha a = \pi \Rightarrow$

$$\Delta E = \frac{\pi^2\hbar^2}{2ma^2}\left[1 - \left(\frac{\alpha a}{\pi}\right)^2\right] = C\,\frac{\pi^2\hbar^2}{2ma^2}$$

P	αa	C	✓ From (b)
0.2	3.0089	0.0827	0.0811
0.5	2.7865	0.2133	0.2026
0.8	2.5288	0.3521	0.3242

(b) According to the problem we are supposed to calculate $\int_0^a V(x)\, e^{2\pi i x/a}\, dx$. The potential we used consisted of a narrow square of width b and depth V_0.



$$\int_0^a V(x)\, e^{2\pi i x/a}\, dx = \int_{a-b}^{a} -V_0\, e^{-2\pi i x/a}\, dx$$

In the limit $b \to 0$ we have $e^{-2\pi i x/a} \simeq \text{constant} = e^{-2\pi i a/a} = 1$

so

$$\int_{a-b}^{a} V(x)\, e^{-2\pi i a x/a}\, dx \simeq -V_0 b$$

and the prediction is

$$\Delta E = \left(\frac{2}{a}\right)(V_0 b)$$

Now P was shorthand for $\beta^2 ab/2$ and $\beta^2 b = \frac{2m}{\hbar^2} bV_0$

$\Rightarrow$

$$P = \left(\frac{a}{2}\right)\left(\frac{2m}{\hbar^2} bV_0\right) \qquad bV_0 = P \cdot \frac{\hbar^2}{ma}.$$

$\Rightarrow$

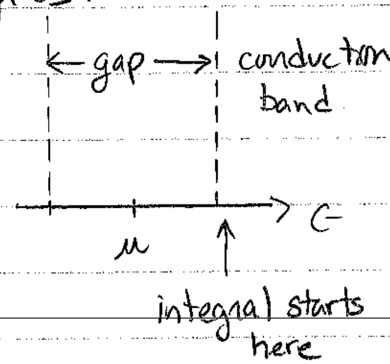
$$\Delta E = \left(\frac{2}{a}\right) P \frac{\hbar^2}{ma} = 4P \frac{\hbar^2}{2ma^2} = \boxed{\left(\frac{4P}{\pi^2}\right) \frac{\pi^2 \hbar^2}{2ma^2}}$$

The predictions are shown in the table on p.3

Overall the agreement is pretty good.

38) To find the number of electrons in the conduction band we just integrate $n(\epsilon)$ over the relevant energies.

$$n(\epsilon) = \frac{g(\epsilon)}{e^{(\epsilon-\mu)/kT}+1}$$



μ is at the center of the gap and so the integral starts at $\epsilon = \frac{1}{2}\Delta E + \mu$ where ΔE is the energy gap. For $g(\epsilon)$ we will use $g(\epsilon) \simeq g(\epsilon_F)$ where $\epsilon_F = 8\text{eV}$.

Then

$$N_{cond} \simeq g(\epsilon_F) \int_{\frac{1}{2}\Delta E+\mu}^{\infty} \frac{1}{e^{(\epsilon-\mu)/kT}+1}\, d\epsilon.$$

Now $\frac{\epsilon-\mu}{kT} \gg 1$ so we can neglect the $+1$ in the denominator.

$$N_{cond} \simeq g(\epsilon_F) \int_{\frac{1}{2}\Delta E+\mu}^{\infty} e^{-(\epsilon-\mu)/kT}\, d\epsilon$$

Let $x = \epsilon - \mu$

$$\Rightarrow \quad N_{cond} \simeq g(\epsilon_F) \int_{\frac{1}{2}\Delta E}^{\infty} e^{-x/kT}\, dx = -kT\, g(\epsilon_F)\, e^{-x/kT}\Big|_{\frac{\Delta E}{2}}^{\infty}$$

$$N_{cond} = kT\, g(\epsilon_F)\, e^{-\Delta E/2kT}$$

For $g(\epsilon_F)$ write $g(\epsilon) = C\epsilon^{1/2}$. The normalization C is found by noting that

$$N_{TOT} = \int_0^{\epsilon_F} g(\epsilon)\, d\epsilon = C \int_0^{\epsilon_F} \epsilon^{\frac{1}{2}}\, d\epsilon$$

$$= C\left(\tfrac{2}{3}\right) \epsilon^{\frac{3}{2}}\Big|_0^{\epsilon_F} = \tfrac{2}{3} C\, \epsilon_F^{\frac{3}{2}}$$

$$\therefore \quad C = \tfrac{3}{2} N_{TOT} / \epsilon_F^{3/2}$$

$$g(\epsilon) = \frac{3}{2} N \frac{\epsilon^{\frac{1}{2}}}{\epsilon_F^{3/2}} \Rightarrow g(\epsilon_F) = \frac{3}{2} \frac{N_{TOT}}{\epsilon_F}$$

$\Rightarrow$

$$\underline{N_{COND} = \frac{3}{2} \frac{kT}{\epsilon_F} e^{-\Delta E/2kT} N_{TOT}}$$

	SILICON	GERMANIUM
ρ	2.33 g/cm^3	5.32 g/cm^3
molecular weight	28.1 g/mole	72.6 g/mole
Density of atoms.	5.0×10^{22}/cm^3	4.4×10^{22}/cm^3
Density of electrons (4/atom)	2.00×10^{23}/cm^3	1.76×10^{23}
ΔE	1.14 eV	0.68 eV.
N_{COND} (@ $kT = .025$ eV)	1.17×10^{11}/cm^3	1.03×10^{15}/cm^3

39) At a density of 0.125 g/cm^3 we have

$$\frac{N}{V} = \frac{0.125\,\text{g/cm}^3}{4\,\text{g/mole}} = 1.88 \times 10^{22}\ \text{atoms/cm}^3 = 18.8\ \text{atoms/nm}^3$$

Now we calculate the number of atoms that can be in the continuum (the excited states). Writing

$$n(\epsilon) = \frac{g(\epsilon)}{e^{\alpha} e^{\epsilon/kT} - 1}$$

with

$$g(\epsilon) = \left(\frac{1}{2\pi}\right)^2 V \left[\frac{2m}{\hbar^2}\right]^{3/2} \epsilon^{\frac{1}{2}}$$

we get

$$N = \int n(\epsilon) d\epsilon = \left(\frac{mkT}{2\pi\hbar^2}\right)^{\frac{3}{2}} V F(\alpha)$$

$F(\alpha)$ has a maximum value $F_{max} = 2.612$ and so the maximum # of atoms that can be in the excited states is

$$\frac{N}{V} = \left(\frac{mkT}{2\pi\hbar^2}\right)^{\frac{3}{2}} F_{max} \qquad m = 4u \simeq 4(938\ MeV/c^2)$$

At $T = 1k$

$$\frac{N}{V} = \left[\frac{4(938\times10^6 eV)(8.617\times10^{-5} eV/k)(1k)}{2\pi\ (197.3\,eV\cdot nm)^2}\right]^{\frac{3}{2}} \cdot 2.612$$

$$= 3.97/nm^3$$

This is the most we can have in the continuum and the rest must be in the ground state

$$\text{Fraction in the g.s} = \frac{18.8 - 3.97}{18.8} = \boxed{79\%}$$