

(a) The conventional bcc unit cell contains 2 atoms, but the primitive unit cell contains only a single atom. Thus sodium, as a monovalent atom, results in a half-filled 1st BZ – and thus gives a metal.

(b) The conventional fcc unit cell contains 4 atoms, but the primitive unit cell contains only one atom. So calcium, which is divalent, could be either a metal or an insulator – depending on the strength of the periodic potential. The fact that it is a metal tells us that the potential is not strong enough to make it an insulator.

(c) C, Si, and Ge are group IV elements and are therefore 4-valent. The fcc unit cell has 4 atoms, but the primitive unit cell has 1 atom, and therefore 4 electrons. This could therefore constitute 2 completely filled bands. In the case of C (diamond) this is indeed an insulator with a large band gap (5.5 eV). For Si and Ge, the band gap is smaller (1.1 eV and .67 eV respectively), hence they are semiconductors.

There are various explanations for this effect. One argument is that for carbon, the periodic potential is extremely strong (no inner shell electrons to screen it, and atoms much closer together) therefore it is an insulator with a large band gap. For Si and Ge, the potential is less strong, so the gap is smaller. Hence they are semiconductors.

Another argument is given by thinking in the tight binding picture. Before you bring the atoms together to make a solid, one needs to consider single-electron orbitals. The higher orbitals in an atom are typically closer together in energy (as they are for hydrogen). For C the valence electrons are in the 2p shell whereas for Si and Ge, the valence electrons are 3p and 4p respectively. Hence we expect smaller gaps for Si and Ge.

In a more chemical language, 4 electrons per atom can therefore form structure. The electrons are all therefore tied up in covalent bonds, making the material an insulator.

Diamond is transparent because it is an insulator with band gap that is larger than any visible light frequency. Thus light cannot be absorbed (or reflected) by any electronic transition.

(b) Effective mass $\hbar^2 k^2 / (2m^*) = (10^{-37} \text{ Joule} \cdot \text{meter}^2) k^2$. So $m^* = 5 \times 10^{-32} \text{ kg}$ or .05 the mass of the electron. This mass is *positive* in the usual convention. The energy is $E = (10^{-37} \text{ Joule} \cdot \text{meter}^2) k^2 = 4 \times 10^{-21} \text{ J}$, or about 0.025 eV. This energy is positive (it takes energy to "push" the hole down into the fermi sea, like pushing a balloon under water).

Getting the momentum and velocity right are tricky. First, note that the velocity of an eigenstate is the same whether or not the state is filled with an electron. It is always true that the velocity of an electron in a state is $\nabla_k E_k / \hbar$ where E_k is the electron energy. Thus the hole velocity here is negative $v = -\hbar k / m^* = -3.8 \times 10^5 \text{ m/s}$ (i.e the velocity is in the negative \hat{x} direction).

For momentum, since a filled band carries no (crystal) momentum, and for electrons crystal momentum is always $\hbar k$, the removal of an electron leaves the band with net momentum $-\hbar k$ which we assign as the momentum of the hole. Thus we obtain hole momentum $-\hbar k = -2.1 \times 10^{-26} \text{ kg} \cdot \text{m/s}$ which is also in the negative \hat{x} direction. (this matches well to the intuition that $p = mv$ with a positive effective mass for holes). With p the density of such holes, the total current density is $pev = -6 \times 10^{-9} \text{ Amp/m}^2$ also in the negative \hat{x} direction (noting that the charge of the hole is positive).

(c) We first calculate the undoped intrinsic carrier concentration using the law of mass action with $n = p = n_{\text{intrinsic}}$. At $T = 293 \text{ Kelvin}$, I obtained

$$n_{\text{intrinsic}} = 10^{16} m^{-3}$$

Then since $n_{\text{dopant}} \gg n_{\text{intrinsic}}$ we can set $p = n_{\text{intrinsic}}^2 / n$ (from the law of mass action) to obtain

$$p = 10^9 m^{-3}$$

Actually this is easy. Using law of mass action $np = n_{\text{intrinsic}}^2$. Thus we write

$$\sigma = e \left(n \mu_e + \frac{n_{\text{intrinsic}}}{n} \mu_h \right)$$

Now set $d\sigma/dn = 0$ to maximize and solve to obtain

$$n = n_{\text{intrinsic}} \sqrt{\mu_h / \mu_e}$$

Which correspondingly results in

$$p = n_{\text{intrinsic}} \sqrt{\mu_e / \mu_h}$$

plugging into the original expression for σ with a tiny bit of algebra we obtain

$$\sigma = 2e n_{\text{intrinsic}} \sqrt{\mu_e \mu_h}$$

as required, and we also obtain

$$n - p = n_{\text{intrinsic}} \left(\sqrt{\mu_h / \mu_e} - \sqrt{\mu_e / \mu_h} \right)$$

Now in the semiconductor quantum wire we must consider the transverse modes. In general the energy of an electron in the wire is then given by

$$E = E_c + \frac{\hbar^2 \pi^2 a_1^2 + a_2^2}{2m_e^* L^2} + \frac{\hbar^2 k^2}{2m_e^*}$$

where a_1 and a_2 are the mode indices (integers greater than zero) in the two transverse directions. Adding the density of states associated with all of these modes we obtain

$$g(E) = \frac{\sqrt{2m_e^*}}{\pi \hbar} \sum_{a_1, a_2 > 0} \left(E - E_c - \frac{\hbar^2 \pi^2 a_1^2 + a_2^2}{2m_e^* L^2} \right)^{-1/2} \Theta \left(E - E_c - \frac{\hbar^2 \pi^2 a_1^2 + a_2^2}{2m_e^* L^2} \right)$$

and similarly in the valence band

$$g(E) = \frac{\sqrt{2m_h^*}}{\pi \hbar} \sum_{a_1, a_2 > 0} \left(E_v - \frac{\hbar^2 \pi^2 a_1^2 + a_2^2}{2m_h^* L^2} - E \right)^{-1/2} \Theta \left(E_v - \frac{\hbar^2 \pi^2 a_1^2 + a_2^2}{2m_h^* L^2} - E \right)$$

(a) This is a particle in a box problem. Both electron and holes are particles in a box of length L . Thus the lowest lying electron in the well is

$$E_e = E_c + \left(\frac{\pi}{L} \right)^2 \frac{\hbar^2}{2m_e^*}$$

with E_c the bulk conduction band minimum. Similarly the highest lying hole state in the well is

$$E_h = E_v - \left(\frac{\pi}{L} \right)^2 \frac{\hbar^2}{2m_h^*}$$

Thus the difference in energy is

$$E_e - E_h = E_{\text{bulkgap}} + \frac{\hbar^2}{2} \left(\frac{\pi}{L} \right)^2 \left(\frac{1}{m_e^*} - \frac{1}{m_h^*} \right)$$

Setting $E_e - E_h - E_{\text{bulkgap}}$ to 1eV and solving for L gives 8 nm.

(b) This type of quantum well device is useful to precisely design a band gap for example for a laser where one wants to fix the emission wavelength. If one puts donor impurities outside of the well (on both sides, say) the donated electrons can reduce their energies by falling into the well, but the ionized dopants remain behind. This is known as modulation doping. It is useful because one can obtain extremely high mobility electrons within the quantum well since there are no ionized dopants in the well to scatter off of. One uses these structures heavily for fundamental physics studies of clean (unperturbed) electrons.

(a) For a 2D electron gas for electrons with mass m , we quickly calculate the density of states.

$$N = 2A \int_0^{k_F} \frac{dk}{(2\pi)^2}$$

with A the area and the factor of 2 out front for spin and \mathbf{k} a two dimensional vector. This can be converted to

$$n = N/A = \frac{k_F^2}{2\pi}$$

When the energy of an electron is given by

$$E = \frac{\hbar^2 \mathbf{k}^2}{2m}$$

we have $k^2 = 2mE/\hbar^2$ and we then have a density of states per unit volume of

$$g = \frac{dn}{dE} = \frac{m}{\pi \hbar^2}$$

This is the correct answer for any $E \geq 0$ and the density of states is zero for any $E < 0$. We then write more precisely that

$$g(E) = \frac{m}{\pi \hbar^2} \Theta(E)$$

where Θ is the step function which has value 1 for nonnegative argument and value 0 for negative argument.

In our quantum well we must make a few minor changes. First of all, we should use the effective mass rather than the actual mass of the electron. Secondly the energy of the particle in the quantum well also includes its particle-in-a-box energy for its motion transverse to the 2D quantum well. Thus for an electron in the conduction band of the quantum well we have

$$E = E_c + \frac{\hbar^2 \pi^2 a^2}{2m_e^* L^2} + \frac{\hbar^2 \mathbf{k}^2}{2m_e^*}$$

where E_c is the bulk conduction band bottom, and $a = 1, 2, 3, \dots$ is the transverse quantum number of the particle in the well. Fixing the transverse quantum number a , the density of states would be

$$g(E) = \frac{m_e^*}{\pi \hbar^2} \Theta \left(E - E_c - \frac{\hbar^2 \pi^2 a^2}{2m_e^* L^2} \right)$$

Now accounting for the fact that there may be many transverse modes we have

$$g(E) = \frac{m_e^*}{\pi \hbar^2} \sum_{a>0} \Theta \left(E - E_c - \frac{\hbar^2 \pi^2 a^2}{2m_e^* L^2} \right)$$

and this expression remains true up to an energy where the transverse modes spill out of the box.

Analogously the density of holes in the valence band in the quantum well is

$$g(E) = \frac{m_h^*}{\pi \hbar^2} \sum_{a>0} \Theta \left(E_v - \frac{\hbar^2 \pi^2 a^2}{2m_h^* L^2} - E \right)$$

(b) First we determine the density of states for a one dimensional electron gas.

$$N = 2L \int_{-k_F}^{k_F} \frac{dk}{2\pi}$$

with L the Length of the system and the factor of 2 out front for spin. This can be converted to

$$n = N/L = \frac{2k_F}{\pi}$$

using $k = \sqrt{2mE}/\hbar$ we then obtain a density of states

$$g(E) = \frac{dn}{dE} = \frac{\sqrt{2m}}{\pi \hbar} E^{-1/2} \Theta(E)$$

(a) A periodic lattice can be thought of as a wave with a reciprocal lattice vector (Bragg diffraction). In the nearly free electron picture, the scattering perturbation is weak, so that we can treat the scattered wave in perturbation theory. In this case, there is an energy denominator which suppresses mixing of k -vectors which have greatly different unperturbed energies. Thus, the only mixing that can occur is between two states with similar energies that are separated by a reciprocal lattice vector. Degenerate perturbation theory tells us that we should first diagonalize within the degenerate space spanned by only these two eigenstates.

(b) We have our (variational) trial wavefunction given by

$$|\psi\rangle = A|k\rangle + B|k+G\rangle \quad (15.2)$$

or equivalently

$$\psi = (Ae^{ikx} + Be^{i(k+G)x})/\sqrt{L}$$

To maintain normalization we can insist that $|A|^2 + |B|^2 = 1$. Taking k and $k+G$ both on a Brillouin zone boundary we have $k = n\pi/a$ and $k+G = -n\pi/a$, where here we have chosen the n^{th} zone boundary, and we must have $G = -2n\pi/a$ the reciprocal lattice vector. The Hamiltonian H in question is the usual Kinetic term plus $V(x)$.

If we simply calculate the expectation value of H in the trial state given by Eq. 15.2 we obtain

$$\langle\psi|H|\psi\rangle = \hbar^2(n\pi/a)^2/(2m) + V_0 + A^*B V_{2n\pi/a} + B^*A V_{2n\pi/a}$$

Using the variational principle, the eigenstate is the trial wavefunction which minimizes the total energy while preserving the normalization. One way to do this is to write $A = \cos(\theta)$ and $B = e^{i\chi} \sin(\theta)$ which is the most general form we can write while still preserving $|A|^2 + |B|^2 = 1$ (we can arbitrarily choose A to be real, since that only introduces an irrelevant overall phase). In terms of these parameters we have

$$\langle\psi|H|\psi\rangle = \hbar^2(n\pi/a)^2/(2m) + V_0 + 2\text{Re}[V_{2n\pi/a} e^{i\chi} \sin(\theta) \cos(\theta)]$$

for $V_{2n\pi/a} > 0$ this is minimized for $\chi = \pi$ and $\theta = \pi/4$ (or equivalently $\chi = 0$ and $\theta = 3\pi/4$). It gives minimum energy states for $\psi = \sin(2n\pi x/a)$ as above.

(c) This calculation is entirely analogous to that above, only here we need to consider k not on the zone boundary. Letting $k = n\pi/a + \delta k$ and $k+G = -n\pi/a + \delta k$ we have

$$\begin{aligned} \langle k|H|k\rangle &= \hbar^2(\delta k + n\pi/a)^2/(2m) + V_0 \\ \langle k+G|H|k+G\rangle &= \hbar^2(\delta k - n\pi/a)^2/(2m) + V_0 \\ \langle k|H|k+G\rangle &= V_{2n\pi/a} \\ \langle k+G|H|k\rangle &= V_{-2n\pi/a} \end{aligned}$$

which we now need to diagonalize. We obtain

$$E_{\pm} = \frac{\hbar^2[(\delta k)^2 + (n\pi/a)^2]}{2m} + V_0 \pm \sqrt{\left[\frac{\hbar^2 2(\delta k)n\pi/a}{2m}\right]^2 + |V_{2n\pi/a}|^2}$$

expanding the square-root we obtain

$$E_{\pm} = \frac{\hbar^2(n\pi/a)^2}{2m} + V_0 \pm |V_{2n\pi/a}| + \frac{\hbar^2(\delta k)^2}{2m} \left(1 \pm \frac{\hbar^2(n\pi/a)^2}{m|V_{2n\pi/a}|}\right)$$

which is a quadratic correction as we move away from the Brillouin zone. Note that for this expansion to remain valid we must have the bracketed term in the square root two equations up small compared to the $|V_{2n\pi/a}|^2$ term.

The effective mass is then obtained by setting

$$\frac{1}{2m^*} = \frac{1}{2m} \left(1 \pm \frac{\hbar^2(n\pi/a)^2}{m|V_{2n\pi/a}|}\right)$$

or equivalently

$$m^* = \left| \frac{m}{1 \pm \frac{\hbar^2(n\pi/a)^2}{m|V_{2n\pi/a}|}} \right|$$

with the + being for the upper band.

Generally we can always write $\rho(\mathbf{x})$ in terms of its Fourier transform

$$\rho(\mathbf{x}) = V \int \frac{d\mathbf{k}}{(2\pi)^3} \rho_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{x}}$$

Now by periodicity we know that $\rho(\mathbf{x}) = \rho(\mathbf{x} + \mathbf{R})$ for any lattice vector \mathbf{R} , so let us take a sum over all N lattice vectors in the system

$$\begin{aligned} \rho(\mathbf{x}) &= \frac{1}{N} \sum_{\mathbf{R}} \rho(\mathbf{x} + \mathbf{R}) = \frac{V}{N} \sum_{\mathbf{R}} \int \frac{d\mathbf{k}}{(2\pi)^3} \rho_{\mathbf{k}} e^{i\mathbf{k}\cdot(\mathbf{x}+\mathbf{R})} \\ &= \frac{V}{N} \int \frac{d\mathbf{k}}{(2\pi)^3} \rho_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{x}} \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} \end{aligned}$$

The sum gives

$$\sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} = \frac{(2\pi)^3}{v} \sum_{\mathbf{G}} \delta^3(\mathbf{k} - \mathbf{G})$$

where the sum is over all \mathbf{G} which are reciprocal lattice vectors and v is the volume of the unit cell. Letting the delta function act and cancelling some factors, we then directly obtain

$$\rho(\mathbf{x}) = \sum_{\mathbf{G}} e^{i\mathbf{G}\cdot\mathbf{x}} \rho_{\mathbf{G}}$$

Here, we can think of the wavevector k as taking an imaginary part (i.e., absorb κ into k)

$$k = -G/2 + i\kappa$$

so that

$$\begin{aligned} \epsilon_0(k) &= \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2((G/2)^2 - iG\kappa - \kappa^2)}{2m} = \epsilon_R - i\epsilon_I \\ \epsilon_0(k+G) &= \frac{\hbar^2(k+G)^2}{2m} = \frac{\hbar^2((G/2)^2 + iG\kappa - \kappa^2)}{2m} = \epsilon_R - i\epsilon_I \end{aligned}$$

where we have defined

$$\begin{aligned} \epsilon_R &= \frac{\hbar^2((G/2)^2 - \kappa^2)}{2m} \\ \epsilon_I &= \frac{\hbar^2(G\kappa)}{2m} \end{aligned}$$

As worked out in the text (Eq. 15.8), the characteristic equation is

$$\begin{aligned} 0 &= (\epsilon_0(k) - E)(\epsilon_0(k+G) - E) - |V_G|^2 \\ &= (\epsilon_R - i\epsilon_I - E)(\epsilon_R + i\epsilon_I - E) - |V_G|^2 \\ &= (\epsilon_R - E)^2 + \epsilon_I^2 - |V_G|^2 \end{aligned} \quad (15.3)$$

Thus, we have

$$E = \epsilon_R \pm \sqrt{|V_G|^2 - \epsilon_I^2}$$

Note here that for $|\epsilon_I| > |V_G|$ the energy becomes imaginary and the solution is not valid. Thus we must have

$$|V_G| \geq |\hbar^2 G\kappa/(2m)|$$

In Eq. 15.3 we have a quadratic equation for κ^2 (there are no lone factors of κ), which can be solved to then give only one (possibly) positive solution

$$\frac{\hbar^2 \kappa^2}{2m} = -\frac{\hbar^2 (G/2)^2}{2m} - E + \sqrt{4E \frac{\hbar^2 (G/2)^2}{2m} + |V_G|^2}$$

In order for this solution to be valid, we must have the right hand side be positive. We can write this condition as

$$\left(\frac{\hbar^2 (G/2)^2}{2m} + E \right)^2 \leq 4E \frac{\hbar^2 (G/2)^2}{2m} + |V_G|^2$$

Or equivalently

$$\left| \frac{\hbar^2 (G/2)^2}{2m} - E \right| \leq |V_G|$$

or in other words, that the energy is inside the gap!

Oops another error in this problem. Actually this one is really bad. The first part of the problem should ask you to show that

$$\psi(x+a) = e^{ika} \psi(x)$$

and it should be ψ that has the form $A \sin(qx) + B \cos(qx)$ not u . Then in the second to last equation there is an extra random factor of k in front of the brackets, it should be q_E not k . AND the exponent is e^{-ika} . Probably too many martinis.

(a) Bloch's theorem tells us

$$\psi(x) = e^{ikx} u(x)$$

with u periodic in the unit cell. This then implies $\psi(x+a) = e^{ika} \psi(x)$ as required.

Between delta functions, there is no potential so the solution must be plane waves $e^{\pm iq_E x}$. Since the Hamiltonian is time reversal invariant we can choose the wavefunction to be real. As a result, we must have ψ of the form $A \sin(q_E x) + B \cos(q_E x)$.

(b) Using $\psi(a^+) = e^{ika} \psi(0) = B e^{ika}$ and $\psi(a^-) = A \sin(q_E a) + B \cos(q_E a)$ gives the required result immediately. The Schroedinger equation evaluated near $x = a$

$$\frac{\hbar^2}{2m} \partial_x^2 \psi(x) = aU \delta(x-a) \psi(x)$$

is equivalent to

$$\frac{\hbar^2}{2m} [\partial_x \psi(a^+) - \partial_x \psi(a^-)] = aU \psi(a)$$

(c) First we note that for $G = \pi/a$, we have

$$V_G = \frac{1}{L} \int dx V(x) e^{iGx} = \frac{1}{L} \sum_n U a = U$$

Note this is true also at $V_0 = U$, so we expect an overall energy shift of U (from V_0) and then a gap of magnitude $2|U|$ opening at the zone boundary as well.

Setting $k = \pi/a$ and $q_E = k + \delta$ we have

$$-1 = \cos(\pm\pi + \delta a) + \frac{mUa}{\hbar^2(\pi/a + \delta)} \sin(\pi + \delta)$$

Expanding for small δ and solving to lowest order we get two solutions

$$\delta = 0 \quad \text{or} \quad \frac{2mUa}{\hbar^2\pi}$$

Substituting back into $E = \hbar^2(\pi/a + \delta)^2/(2m)$ we obtain

$$E = E_0 \quad \text{or} \quad E_0 + 2U$$

giving the gap of $2|U|$ at the zone boundary as expected (and the mid-point of the gap shifted up by U due to V_0 as well).

Using

$$\begin{aligned} \psi(a) &= B e^{ika} \\ \partial_x \psi(a^+) &= e^{ika} q_E A \\ \partial_x \psi(a^-) &= q_E [A \cos(q_E a) - B \sin(q_E a)] \end{aligned}$$

gives the desired result which now reads (after removing errors!)

$$A - e^{-ika} [A \cos(q_E a) - B \sin(q_E a)] = 2maUB/(q_E \hbar^2)$$

The two equations (with errors removed) have the required solution.