

1 (a) For any particle moving in a potential, there is an associated wavefunction, ψ , which is a function of space coordinates and time. The wavefunction determines everything that can be known about the particle. Specific information, such as the kinetic energy of the particle, may be determined by applying an operator to the wavefunction [5%]. The basic postulates of quantum mechanics require that the wavefunction must satisfy the Schrödinger Equation at all times [5%], that the wavefunction must be single-valued for all space and time coordinates and that both the wavefunction and its first derivative of any space coordinate must be continuous [5%]. The probability, P , of finding the particle in a volume element d^3V is then given by

$$Pd^3V = |\psi|^2 d^3V \quad [5\%]$$

(b) From the form of the wavefunction given, we can determine that

$$\frac{d\psi}{dx} = -A_0\alpha^2 x \exp\left(\frac{-\alpha^2 x^2}{2}\right) \quad [5\%]$$

and

$$\frac{d^2\psi}{dx^2} = A_0\alpha^2(\alpha^2 x^2 - 1)\exp\left(\frac{-\alpha^2 x^2}{2}\right) \quad [5\%]$$

For this wavefunction to be valid, it must satisfy the time independent Schrödinger equation,

$$\frac{-\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V\psi = E\psi \quad [10\%]$$

Substitution from above gives

$$E\psi = A_0 \exp\left(\frac{-\alpha^2 x^2}{2}\right) \left\{ \frac{\hbar^2 \alpha^2}{2m} + \left(\frac{c}{2} - \frac{\hbar^2 \alpha^4}{2m} \right) x^2 \right\} \quad [15\%]$$

Only if

$$\alpha^2 = \frac{(cm)^{1/2}}{\hbar}$$

does the x^2 coefficient equal 0 and the time independent Schrödinger equation is satisfied [10%].

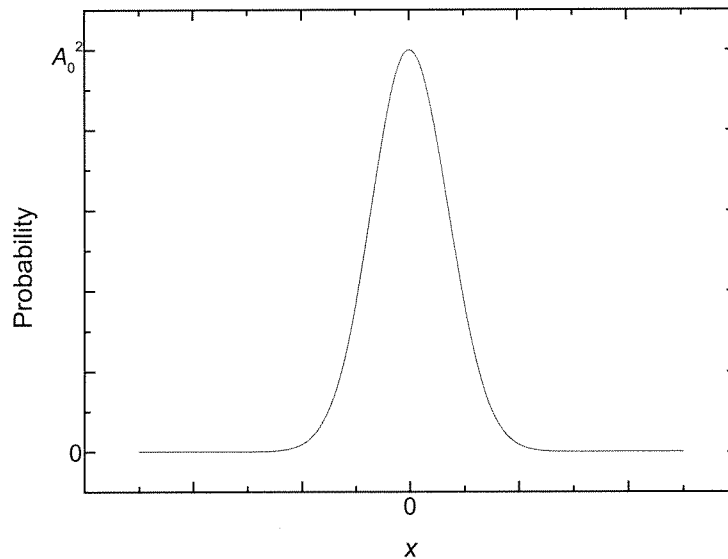
It can then be seen that

$$E = \frac{\hbar^2 \alpha^2}{2m} \quad [5\%]$$

Substituting for α gives the final expression for the total energy of the particle,

$$E = \frac{\hbar}{2} \left(\frac{c}{m} \right)^{1/2} \quad [5\%]$$

(c) The probability of finding the particle varies as $|\psi|^2$. Hence, the sketch of the probability distribution is shown below.



[10%]

This distribution differs from the classical description in several respects:

- The 'wings' of the distribution extend beyond the classical extent of the oscillation [5%].
- The energy of the ground state is zero in the classical description, which is not the case here [5%].
- Given that the energy is non-zero, in the classical description, the particle has greatest velocity at $x = 0$ and zero velocity when $|x|$ is maximised, and so the most probable position for the particle is also when $|x|$ is maximised and is least at $x = 0$, whilst the reverse is true in the quantum mechanical description [5%].

- 2 (a) The Free Electron Theory assumes that
- Electrons in the solid behave like a gas of free particles which are free to move in the solid [5%].
 - Removal of a valence electron to be a free carrier leaves behind a positively charged ion core, and the associated charge density due to these ion cores is spread uniformly throughout the solid [5%].
 - There is no interaction between free electrons [5%].

(b) The average electron energy is given by the total energy of all the electrons divided by the number of free electrons, so

$$\langle E \rangle = \frac{1}{N} \int_0^{\infty} E n(E) dE = \frac{1}{N} \int_0^{\infty} E g(E) f(E) dE \quad [10\%]$$

At absolute zero, the Fermi function is 1 below E_F and zero above E_F , so this becomes

$$\langle E \rangle = \frac{1}{N} \int_0^{E_F} E g(E) dE \quad [5\%]$$

Therefore, substituting for the energy density of states,

$$\begin{aligned} \langle E \rangle &= \frac{1}{N} \int_0^{E_F} E \frac{V}{2\pi^2 \hbar^3} (2m)^{3/2} E^{1/2} dE \\ &= \frac{V (2m)^{3/2}}{N 2\pi^2 \hbar^3} \int_0^{E_F} E^{3/2} dE \quad [10\%] \\ \langle E \rangle &= \frac{V (2m)^{3/2}}{N 5\pi^2 \hbar^3} E_F^{5/2} \end{aligned}$$

(c) The number density of electrons in a system may be calculated from the density of states by

$$\begin{aligned} \frac{N}{V} &= \frac{1}{V} \int_0^{E_F} g(E) dE \\ &= \frac{1}{2\pi^2 \hbar^3} (2m)^{3/2} \int_0^{E_F} E^{1/2} dE \quad [15\%] \\ \frac{N}{V} &= \frac{1}{2\pi^2 \hbar^3} (2m)^{3/2} \frac{2E_F^{3/2}}{3} \end{aligned}$$

Substituting into the equation for $\langle E \rangle$ gives

$$\langle E \rangle = \frac{3E_F}{5} \quad [10\%]$$

(d) Rearranging the expression for N/V gives

$$E_F = \frac{\hbar^2}{2m} \left(3\pi^2 \frac{N}{V} \right)^{2/3} \quad [5\%]$$

Hence, assuming that for a Group I metal each atom gives up one free electron [5%], we have that

$$\begin{aligned} \langle E \rangle &= \frac{3E_F}{5} \\ &= \frac{3\hbar^2}{10m} \left(3\pi^2 \frac{N}{V} \right)^{2/3} \\ &= \frac{3(1.055 \times 10^{-34})^2}{10.9 \cdot 109 \times 10^{-31}} (3\pi^2 \cdot 2.54 \times 10^{28})^{2/3} \\ \langle E \rangle &= 3.032 \times 10^{-19} \text{ J} = 1.89 \text{ eV} \end{aligned} \quad [10\%]$$

The wavenumber may be calculated from the energy of a free electron by

$$\begin{aligned} k &= \frac{(2mE)^{1/2}}{\hbar} \\ &= \frac{(2.9 \cdot 109 \times 10^{-31} \cdot 3.032 \times 10^{-19})^{1/2}}{1.055 \times 10^{-34}} \\ k &= 7.04 \times 10^9 \text{ m}^{-1} \end{aligned} \quad [10\%]$$

The wavelength is then related to the wavenumber by

$$\begin{aligned} \lambda &= \frac{2\pi}{k} \\ \lambda &= 8.92 \times 10^{-10} \text{ m} \end{aligned} \quad [5\%]$$

3 (a) Let us consider the unoccupied states at the top of the VB in detail. If we remove a single electron from the VB with a wavenumber k_e then we know that the sum of the wavenumber for all of the remaining electrons will be $-k_e$. Therefore, we can consider this absence of an electron to be a **hole** of wavenumber k_h where

$$k_h = -k_e \quad [5\%]$$

The hole is simply a **hypothetical** particle which represents the absence of an electron from a state in a convenient fashion. If the energy of the electron occupying the state before removal was E_e , then the energy of the hole, E_h , must be

$$E_h = -E_e \quad [5\%]$$

Hence, the group velocity of the hole, v_h , is

$$v_h = \frac{dE_h}{dk_h} = \frac{d(-E_e)}{d(-k_e)} = v_e \quad [5\%]$$

where v_e is the group velocity of the electron that previously occupied the state.

From Eqn. 6.14 in the lecture notes, the effective mass of the hole is

$$m_h^* = \frac{\hbar^2}{d^2 E_h / dk_h^2} = \frac{-\hbar^2}{d^2 E_e / dk_e^2} = -m_e^* \quad [5\%]$$

The application of an electric field, \mathcal{E} , will cause a change in hole momentum, p_h

$$F = \frac{dp_h}{dt} = \frac{\hbar dk_h}{dt} = \frac{-\hbar dk_e}{dt} = -(-e\mathcal{E}) = e\mathcal{E} \quad [5\%]$$

The hole behaves as though it has a **positive charge** of $+e$.

(b) (i) Assuming that all acceptors are ionised [5%] then

$$\begin{aligned} N_A &= p \\ &= N_V \exp\left(\frac{-E_F}{kT}\right) \\ &= 7 \times 10^{24} \exp\left(\frac{-0.05}{0.862 \times 10^{-4} \cdot 298}\right) \\ N_A &= 1 \times 10^{24} \text{ m}^{-3} \end{aligned} \quad [5\%]$$

(ii) From the Law of Mass Action, we know that

$$n_i^2 = N_C N_V \exp\left(\frac{-E_C}{kT}\right) \quad [5\%]$$

Hence, the effective density of states in the conduction band may be found,

$$\begin{aligned} N_C &= \frac{n_i^2}{N_V} \exp\left(\frac{E_C}{kT}\right) \\ &= \frac{(10^{16})^2}{7 \times 10^{24}} \exp\left(\frac{1.1}{0.862 \times 10^{-4} \cdot 298}\right) \quad [5\%] \\ N_C &= 5.65 \times 10^{25} \text{ m}^{-3} \end{aligned}$$

From this, the density of donors may be found, again assuming that all are ionised

$$\begin{aligned} N_D &= n \\ E_F - E_C &= kT \ln\left(\frac{N_D}{N_C}\right) \quad [5\%] \\ &= 0.862 \times 10^{-4} \cdot 298 \ln\left(\frac{10^{24}}{5.65 \times 10^{25}}\right) \\ E_F - E_C &= -0.10 \text{ eV} \end{aligned}$$

(c) Consider the p-type side of the junction. The Poisson equation states that

$$\nabla^2 V = \frac{-\rho}{\epsilon_0 \epsilon_r} = \frac{-eN_A}{\epsilon_0 \epsilon_r}$$

Given that V only varies in the x direction, then

$$\frac{d^2 V}{dx^2} = \frac{-eN_A}{\epsilon_0 \epsilon_r} \quad [10\%]$$

Integrating the equation gives the general solution,

$$\frac{dV}{dx} = \frac{-eN_A x}{\epsilon_0 \epsilon_r} + C$$

We know that at $x=w_p$ the electric field is zero, so

$$C = \frac{eN_A w_p}{\epsilon_0 \epsilon_r}$$

and hence,

$$\frac{dV}{dx} = \frac{eN_A(w_p - x)}{\epsilon_0 \epsilon_r} \quad [10\%]$$

Integrating again gives the general solution,

$$V = \frac{eN_A}{\epsilon_0 \epsilon_r} \left(K + w_p x - \frac{x^2}{2} \right)$$

We can make $x = 0$ our arbitrary reference point, and set V at this point to be zero, so $K = 0$ and then the voltage on the p-side, V_p is simply the potential at $x = w_p$, so

$$V_p = \frac{eN_A w_p^2}{2\epsilon_0 \epsilon_r} \quad [10\%]$$

As the n-type side of the junction has an equal doping density, then the width of the junction on the n side must be the same, as must be the potential difference, so

$$V_p = \frac{eN_A w_p^2}{2\epsilon_0 \epsilon_r} = V_n = \frac{eN_D w_n^2}{2\epsilon_0 \epsilon_r} = \frac{V_0}{2} \quad [5\%]$$

Hence,

$$w = 2w_p = 2 \left(\frac{\epsilon_0 \epsilon_r V_0}{eN_A} \right)^{1/2} \quad [5\%]$$

as required.

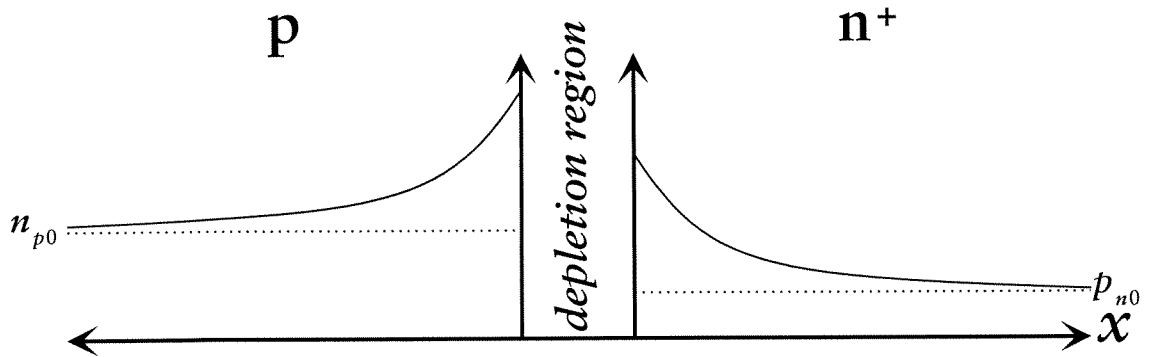
For a pn junction,

$$eV_0 = E_{Fn} - E_{Fp} = E_C + (E_{fn} - E_C) - E_{fp} = 1 \cdot 10 + (-0 \cdot 10) - 0 \cdot 05 = 0 \cdot 95 \text{ eV} \quad [5\%]$$

Hence,

$$w = 2 \left(\frac{\epsilon_0 \epsilon_r V_0}{e N_A} \right)^{1/2}$$
$$= 2 \left(\frac{8.854 \times 10^{-12} \cdot 12.0 \cdot 95}{1.602 \times 10^{-19} \cdot 10^{24}} \right)^{1/2} \quad [5\%]$$
$$w = 50 \text{ nm}$$

4 (a)



[20%]

(b) We assume that the injected concentration of minority carriers is much less than the majority carrier concentration, that no recombination takes place in the depletion region and that the electric field outside the depletion region is negligible.

[10%]

The Continuity Equation states that

$$\frac{\partial(p - p_{n0})}{\partial t} = -\frac{(p - p_{n0})}{\tau_h} - \mu_h E \frac{\partial(p - p_{n0})}{\partial x} + D_h \frac{\partial^2(p - p_{n0})}{\partial x^2}$$

[5%]

In steady state, we know that

$$\frac{\partial(p - p_{n0})}{\partial t} = 0$$

and that there is no E-field outside the junction so

$$\mu_h E \frac{\partial(p - p_{n0})}{\partial x} = 0$$

[5%]

Hence,

$$D_h \frac{\partial^2 p}{\partial x^2} = \frac{p - p_{n0}}{\tau_h}$$

[5%]

where p_{n0} is the intrinsic minority carrier concentration, which is independent of position and τ_h is the minority carrier lifetime. This has the general solution

$$p - p_{n0} = A \exp\left(\frac{-x}{L_h}\right) + B \exp\left(\frac{x}{L_h}\right)$$

[5%]

where L_h is the hole diffusion length given by

$$L_h^2 = D_h \tau_h$$

We know that $p - p_{n0} \rightarrow 0$ as $x \rightarrow \infty$ and so $B=0$ and the solution to the diffusion equation becomes

$$p - p_{n0} = A \exp\left(\frac{-x}{L_h}\right)$$

[5%]

We need to find the constant A using the boundary condition that the number of holes (at $x=0$) being injected across the junction under forward bias is

$$p(x=0) = p_{n0} \exp\left(\frac{eV}{kT}\right) = A + p_{n0}$$

[5%]

Hence, substituting for A gives the required result that

$$p - p_{n0} = p_{n0} \left[\exp\left(\frac{eV}{kT}\right) - 1 \right] \exp\left(\frac{-x}{L_h}\right)$$

[5%]

(c) The current due to hole diffusion is given by

$$I_h = -AeD_h \left. \frac{\partial p}{\partial x} \right|_{x=0}$$

[5%]

where A is the area of the junction. Substituting for the result from part (b),

$$I_h = -AeD_h \frac{p_{n0}}{L_h} \left[\exp\left(\frac{eV}{kT}\right) - 1 \right]$$

$$I_h = I_{sh} \left[\exp\left(\frac{eV}{kT}\right) - 1 \right]$$

where

$$I_{sh} = Ae \left(\frac{D_h}{L_h} \right) p_{n0}$$

[10%]

Similarly, for electrons on the p-side of the junction,

$$I_e = I_{se} \left[\exp \left(\frac{eV}{kT} \right) - 1 \right]$$

where

$$I_{se} = Ae \left(\frac{D_e}{L_e} \right) n_{p0}$$

[5%]

Hence, the total current flow is

$$I = I_h + I_e = I_s \left[\exp \left(\frac{eV}{kT} \right) - 1 \right]$$

[5%]

The reverse saturation current is

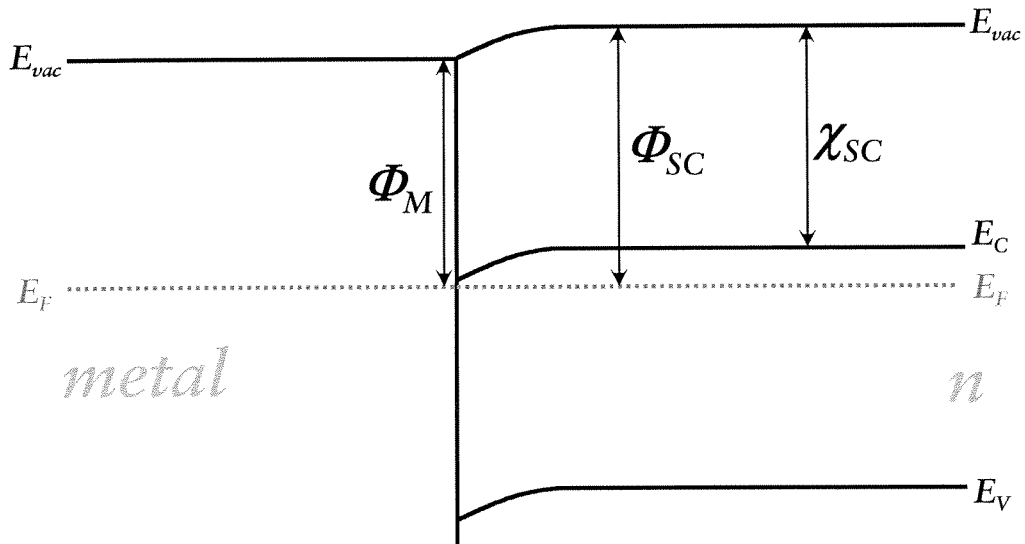
$$I_s = Ae \left(\frac{D_e n_{p0}}{L_e} + \frac{D_h p_{n0}}{L_h} \right)$$

but knowing that $L_h^2 = D_h \tau_h$ this becomes

$$I_s = Ae \left(\frac{L_e n_{p0}}{\tau_e} + \frac{L_h p_{n0}}{\tau_h} \right)$$

[10%]

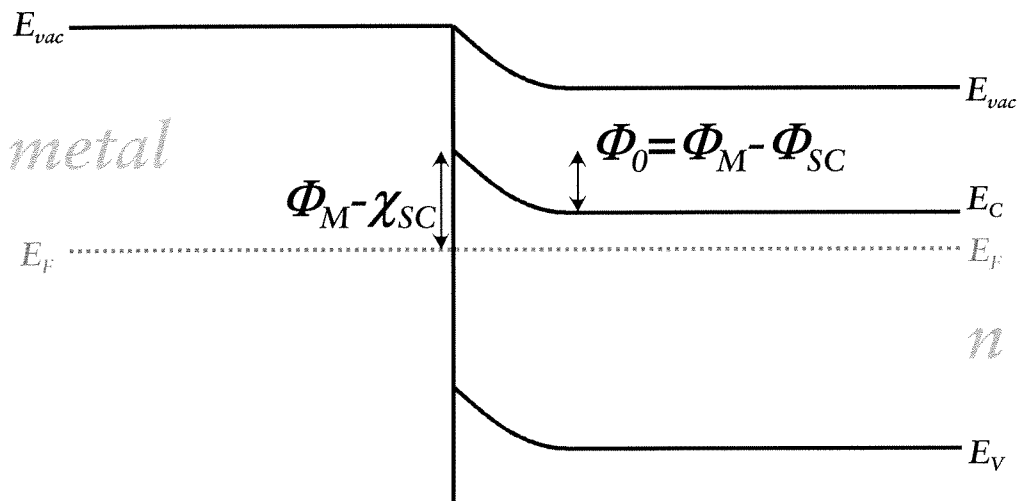
5 (a) Consider an n-type semiconductor-metal junction. If the work function of the metal ϕ_m is less than that of the semiconductor ϕ_{sc} then we get the following band diagram



If a positive bias is applied to the metal, there is no barrier to electron flow from the s/c into the metal. Similarly, there is almost no barrier to electron flow from the metal into the s/c if a negative bias is applied to the metal. Therefore, this situation produces an Ohmic contact.

[10%]

However, if $\phi_m > \phi_{sc}$ then the following band structure results.



Now if a positive bias is applied to the metal, the band bending must first be overcome before current will flow in the form of electrons from the s/c into the metal. If a negative

bias is applied to the metal, then there is a constant large barrier to electron flow from the metal into the s/c and very little current will flow. A Schottky Barrier Diode results. [20%]

(b) (i) For an n-type semiconductor

$$n = N_C \exp\left(\frac{E_F - E_C}{kT}\right) \approx N_D$$

$$E_F - E_C = kT \ln\left(\frac{N_D}{N_C}\right)$$

$$= 0.862 \times 10^{-4} \cdot 298 \cdot \ln\left(\frac{5 \times 10^{22}}{4 \times 10^{25}}\right)$$

$$E_F - E_C = -0.172 \text{ eV}$$

[10%]

Therefore, the silicon workfunction is

$$\phi_{\text{Si}} = \chi + (E_C - E_F)$$

$$= 4.05 + 0.17$$

$$\phi_{\text{Si}} = 4.22 \text{ eV}$$

[5%]

We know that ϕ_m is 4.7 eV, so this is a Schottky Barrier, where the barrier to electron flow from the Si to the metal is the degree of band bending of the conduction band which is

$$\text{Barrier}_{\text{Si} \rightarrow \text{m}} = \phi_m - \phi_{\text{Si}}$$

$$= 4.70 - 4.22$$

$$\text{Barrier}_{\text{Si} \rightarrow \text{m}} = 0.48 \text{ eV}$$

[10%]

(ii) The barrier to electron flow from the metal to the Si is the band bending plus $E_C - E_F$, so

$$\text{Barrier}_{\text{m} \rightarrow \text{Si}} = \phi_m - \phi_{\text{Si}} + (E_C - E_F)$$

$$= 4.70 - 4.22 + 0.17$$

$$\text{Barrier}_{\text{m} \rightarrow \text{Si}} = 0.65 \text{ eV}$$

[15%]

(iii) The current is given by the Richardson-Dushman equation (with no corrections as we can use the free electron mass) where the barrier term is that from the metal to the semiconductor [10%] and hence,

$$\begin{aligned} I &= AT^2 \exp\left(\frac{-\phi_{m \rightarrow Si}}{kT}\right) \\ &= \pi(0.125 \times 10^{-3})^2 \cdot 1.204 \times 10^6 \cdot 298^2 \cdot \exp\left(\frac{-0.65}{0.862 \times 10^{-4} \cdot 298}\right) \\ I &= 53.7 \text{ nA} \end{aligned}$$

[20%]