**Worked solutions**

**Semiconductor Engineering 3B5 Examination 2016**

**Question 1**
   (a) Take the time-dependent Schrödinger equation and substitute in the functions for $V(x)$ and $\Psi(x,t)$:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V\Psi = j\hbar\frac{\partial}{\partial t}\Psi$$

$$\therefore -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\left(A\exp\left(-\frac{\sqrt{km}}{2\hbar}x^2\right)\exp(-j\omega t)\right)$$

$$+k\frac{x^2}{2}\left(A\exp\left(-\frac{\sqrt{km}}{2\hbar}x^2\right)\exp(-j\omega t)\right)$$

$$= j\hbar\frac{\partial}{\partial t}\left(A\exp\left(-\frac{\sqrt{km}}{2\hbar}x^2\right)\exp(-j\omega t)\right)$$

$$\therefore -\frac{\hbar^2}{2m}\frac{\partial}{\partial x}\left(\left[-x\frac{\sqrt{km}}{\hbar}\right]\exp\left(-\frac{\sqrt{km}}{2\hbar}x^2\right)\right)+k\frac{x^2}{2}\left(\exp\left(-\frac{\sqrt{km}}{2\hbar}x^2\right)\right)$$

$$= (-j\omega)j\hbar\left(\exp\left(-\frac{\sqrt{km}}{2\hbar}x^2\right)\right)$$

$$\therefore -\frac{\hbar^2}{2m}\left(\left[-\frac{\sqrt{km}}{\hbar}\right]\exp\left(-\frac{\sqrt{km}}{2\hbar}x^2\right)+\left[-x\frac{\sqrt{km}}{\hbar}\right]^2\exp\left(-\frac{\sqrt{km}}{2\hbar}x^2\right)\right)$$

$$+k\frac{x^2}{2}\left(\exp\left(-\frac{\sqrt{km}}{2\hbar}x^2\right)\right)=\omega\hbar\left(\exp\left(-\frac{\sqrt{km}}{2\hbar}x^2\right)\right)$$

$$\therefore -\frac{\hbar^2}{2m}\left(\left[-\frac{\sqrt{km}}{\hbar}\right]+\left[-x\frac{\sqrt{km}}{\hbar}\right]^2\right)+k\frac{x^2}{2}=\omega\hbar$$

$$\therefore -\frac{\hbar^2}{2m}\left(-\frac{\sqrt{km}}{\hbar}\right)-\frac{\hbar^2}{2m}\left[-x\frac{\sqrt{km}}{\hbar}\right]^2+k\frac{x^2}{2}=\omega\hbar$$

$$\therefore \frac{\hbar\sqrt{k}}{2\sqrt{m}}-\frac{\hbar^2}{2m}\left[-x\frac{\sqrt{km}}{\hbar}\right]^2+k\frac{x^2}{2}=\omega\hbar$$

$$\therefore \frac{\hbar\sqrt{k}}{2\sqrt{m}}-k\frac{x^2}{2}+k\frac{x^2}{2}=\omega\hbar$$

$$\therefore \frac{\sqrt{k}}{2\sqrt{m}}=\omega$$

[30%]

(b) The time-dependent part is characterised by frequency $= \frac{\sqrt{k}}{2\sqrt{m}}$ .

In terms of cycles per second, the frequency is given by $\nu = \frac{\sqrt{k/m}}{4\pi}$.

The energy is calculated from the de-Broglie–Einstein relationship:
$$E_0 = h\nu = h\frac{\sqrt{k/m}}{4\pi} = \hbar\omega = \hbar\frac{\sqrt{k/m}}{2}.$$

There is an alternative way of calculating the total energy. This assumes that the potential energy $V(x)$ is zero (i.e. by evaluating at $x = 0$) and the total energy equals the kinetic energy. We then use the kinetic energy operator $T = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$ on the wave function $\Psi$. This will also yield $\frac{\hbar\sqrt{k}}{2\sqrt{m}}$.

[10%]

(c) The uncertainty in the electron's position is given by

$$\Delta x = 2\hbar^{1/2}/(km)^{1/4}$$

Heisenberg's uncertainty principle is given by

$$\Delta x \Delta p \geq \frac{\hbar}{2}$$
$$\therefore \Delta p \geq \frac{\hbar}{2\Delta x} = \frac{\hbar}{4\hbar^{1/2}/(km)^{1/4}} = \frac{\hbar^{1/2}(km)^{1/4}}{4}$$

This allows the minimum kinetic energy, $T$, of the electron to be calculated:
$$T = \frac{p^2}{2m}$$
$$\therefore T_{min} = \frac{(\Delta p)^2}{2m} = \frac{1}{2m}\left(\frac{\hbar^{1/2}(km)^{1/4}}{4}\right)^2 = \frac{\hbar\sqrt{k/m}}{32}$$

In part (ii) we calculated the ground state energy as $E_0 = \hbar\frac{\sqrt{k/m}}{2}$. This is higher than the minimum kinetic energy $T$, and therefore entirely compatible with the uncertainty principle. The momentum of the electron will always be above the minimum required by the Heisenberg uncertainty principle.

[20%]

(d) The quantum mechanical effect of tunnelling means that the electron's wave function can extend beyond the boundaries of the well even if the energy of the state is lower than the energy of the barrier.

$V(x)=k\,x^2/2$

$\Psi_2$

$E_2$

$\Psi_1$

$E_1$

tunnelling

$\Psi_0$

$E_0$

$x$

$0$
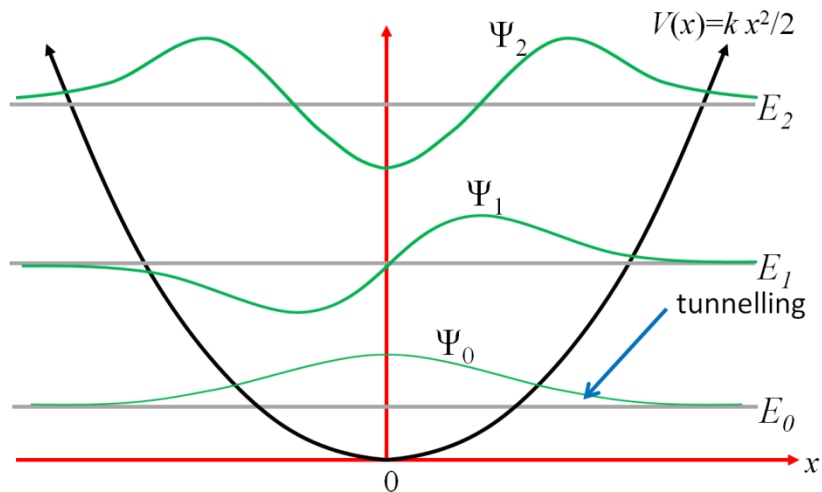
[25%]

(e) As the wells are brought closer, the wave functions of the highest occupied energy levels spatially extend across the two wells. The Pauli exclusion principle is invoked which states that two electrons cannot exist in the same state. Their wave functions therefore become perturbed and their energy levels split into two.

[15%]

**Question 2**

(a) Boltzmann statistics apply when multiple particles can exist in the same state. Electrons, however, obey the Pauli exclusion principle, which states that no two electrons can occupy the same quantum mechanical state. In this case, Boltzmann statistics are not appropriate and Fermi-Dirac statistics should be used. Fermi-Dirac statistics account for the fact that electrons tend to occupy the lowest available energy state, and (because no two electrons can occupy the same state) that the electrons are forced to occupy higher and higher energy levels as the lower energy levels fill up. For low probability of occupation ($E \gg E_F$) the Fermi function approaches a Boltzmann distribution.

From a physicist's perspective, electrons are "fermions" with half-integer spin. Fermions obey the Pauli exclusion principle, and hence follow Fermi-Dirac statistics.

[15%]

(b) Above zero Kelvin, we consider the Fermi energy to be the energy at which there is a 50% probability that a state is occupied. (This is actually an approximation that is valid provided $E_F \gg kT$.)

At zero Kelvin, the Fermi energy is the highest occupied energy level. [15%]

(c)

$p$ is the number density of holes in the VB:

$$p = \frac{1}{V}\int_{-\infty}^{E_V} g(E)f_p(E)\,\mathrm{d}E$$

$$= \frac{1}{V}\int_{-\infty}^{E_V} g(E)[1 - f(E)]\,\mathrm{d}E$$

If $E_F - E_V \gg kT$, then we may again use the Boltzmann distribution as an approximation for the Fermi function, so:

$$f_p(E) = e^{\left(\frac{E-E_F}{kT}\right)}$$

Substituting gives:

$$p = \frac{1}{V} \int_{-\infty}^{E_V} g(E) f_p(E) \, dE$$

$$= \frac{1}{V} \int_{-\infty}^{E_V} \frac{V}{2\pi^2 \hbar^3} (2m_h^*)^{\frac{3}{2}} (E_V - E)^{\frac{1}{2}} e^{\left(\frac{E-E_F}{kT}\right)} \, dE$$

$$= \int_{-\infty}^{E_V} \frac{(2m_h^*)^{\frac{3}{2}}}{2\pi^2 \hbar^3} (E_V - E)^{\frac{1}{2}} e^{\left(\frac{E-E_F}{kT}\right)} \, dE$$

$$= \int_{-\infty}^{E_V} \frac{(2m_h^*)^{\frac{3}{2}}}{2\pi^2 \hbar^3} (E_V - E)^{\frac{1}{2}} e^{\left(\frac{-(E_V-E)-(E_F-E_V)}{kT}\right)} \, dE$$

To solve this, we substitute $x = (E_V - E)^{\frac{1}{2}}$, so:

$$p = \frac{(2m_h^*)^{\frac{3}{2}}}{2\pi^2 \hbar^3} e^{\left(\frac{-(E_F-E_V)}{kT}\right)} \int_0^{\infty} x e^{\left(\frac{-x^2}{kT}\right)} 2x \, dx$$

and use the standard integral to obtain:

$$p = \frac{(2m_h^*)^{\frac{3}{2}}}{2\pi^2 \hbar^3} e^{\left(\frac{-(E_F-E_V)}{kT}\right)} \frac{1}{2} \sqrt{\pi (kT)^3}$$

$$= 2 \left(\frac{m_h^* kT}{2\pi \hbar^2}\right)^{\frac{3}{2}} e^{\left(\frac{-(E_F-E_V)}{kT}\right)}$$

This can be rewritten to give:

$$p = N_V e^{\left(\frac{-(E_F-E_V)}{kT}\right)}$$

where

$$N_V = 2 \left(\frac{m_h^* kT}{2\pi \hbar^2}\right)^{\frac{3}{2}}$$

[30%]

(d)
    (i)
Due to electrical neutrality of the semiconductor, we can write:
$$p + (N_D - n_D) = n + (N_A - p_A)$$

Assuming that there are no donors ($N_D = 0, n_D = 0$), that the number of electrons generated due to thermal excitation for the VB to the CB is negligible ($n = 0$), and that all Zn acceptors are fully ionised at 290 K ($p_A = 0$), we obtain:
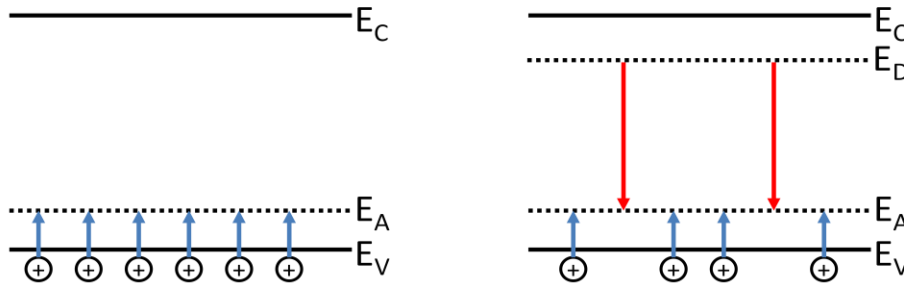
$$p = N_A$$

Rearranging $p = N_V e^{\left(\frac{-(E_F - E_V)}{kT}\right)}$ and substituting $p = N_A$ gives

$$E_F - E_V = kT\ln\left(\frac{N_V}{N_A}\right)$$

$$= 0.025 \times \ln\left(\frac{9.0 \times 10^{18}}{1.0 \times 10^{17}}\right)$$

$$= 0.11 \text{ eV}$$

$$= 110 \text{ meV} \qquad\qquad\qquad\qquad\qquad\qquad [15\%]$$

(ii)



If there are only acceptors present, these accept electrons from the valence band. Vacant states knowns as holes are left behind in the valence band.

If there are donors present also, their electrons are released. Their electrons can fall into the acceptor states. This ionises the acceptors without yielding a free hole in the valence band.

The semiconductor now contains both acceptors and donors. When the donors are ionised, their electrons are released. These electrons fall into the acceptor states. This ionises the acceptor without yielding a free hole in the valence band. The resulting hole density is approximately equal to the difference between the acceptor and donor concentration.

Due to electrical neutrality of the semiconductor, we can write:

$$p + (N_D - n_D) = n + (N_A - p_A)$$

Assuming that all donors are ionised ($N_D = 2 \times 10^{16}$, $n_D = 0$), that the number of electrons generated due to thermal excitation for the VB to the CB is negligible, and all Zn acceptors are fully ionised at room temperature ($N_A = 1 \times 10^{17}$, $p_A = 0$), we obtain:

$$p + (N_D - n_D) = n + (N_A - p_A)$$
$$\therefore p + (2 \times 10^{16}) = n + (1 \times 10^{17})$$
$$\therefore p = n + (1 \times 10^{17} - 2 \times 10^{16})$$
$$= n + 8 \times 10^{16}$$

Now,

$$np = n_i^2$$

So

$$p = \frac{n_i^2}{p} + 8 \times 10^{16}$$

$$\therefore p^2 - (8 \times 10^{16})p - n_i^2 = 0$$
$$\therefore p^2 - (8 \times 10^{16})p - (2.1 \times 10^6)^2 = 0$$

Solving the quadratic equation gives

$$\therefore p = \frac{(8 \times 10^{16})}{2} + \sqrt{\frac{(8 \times 10^{16})^2 + 4(2.1 \times 10^6)^2}{2}}$$
$$\approx 8 \times 10^{16} \text{cm}^{-3}$$

The resulting hole density is approximately equal to the difference between the acceptor and donor concentration. This is the majority carrier density.
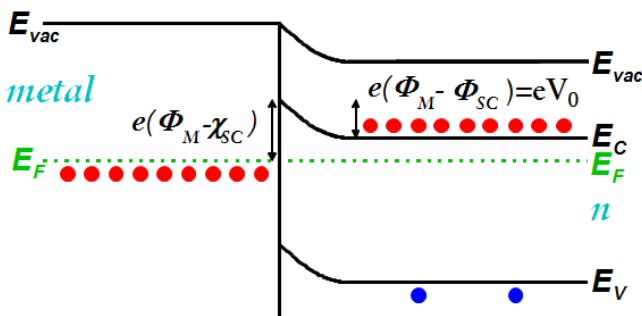
$$np = n_i^2$$
$$\therefore n = \frac{n_i^2}{p} = \frac{(2.1 \times 10^6)^2}{8 \times 10^{16}} = 0$$

The minority carrier density is essentially zero. [25%]

**Question 3**
(a) (i)



[10%]

(ii) $e\Phi_{SC} = 4.2eV = e\chi + (E_C - E_F)$

Hence $(E_C - E_F) = 0.15eV$

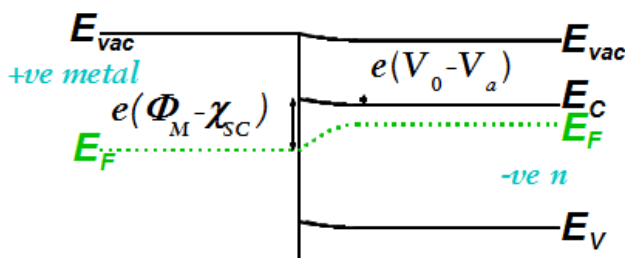Assuming all donor atoms are fully ionised :
$$n = N_D = N_C \exp\left(\frac{E_F - E_C}{kT}\right) = 2.8 \times 10^{25} \exp\left(\frac{-0.15}{0.025}\right) = 6.94 \times 10^{22} \text{m}^{-3}$$

[20%]

(iii) Built-in (contact) potential can be measured by CV measurements in reverse bias (see 3B5 lab and 3B5 example paper 3 - Q3) or for instance photothermal measurements. Note it cannot be directly measured with voltmeter.
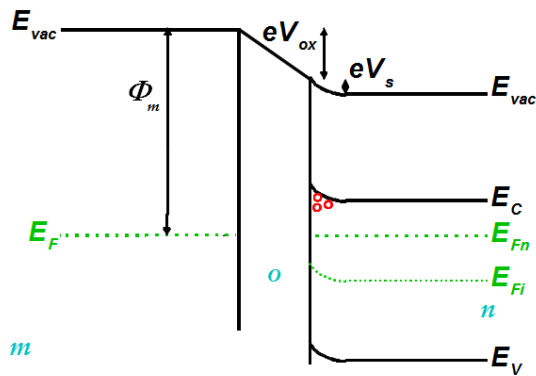
[10%]

(b) (i)



[10%]

(ii) $V_B = \Phi_M - \chi_{SC} = 4.9V - 4.05V = 0.85V$ [10%]

(iii) $J_{s-m} = AT^2 \exp\left(\dfrac{-eV_b}{kT}\right)\exp\left(\dfrac{eV_a}{kT}\right)$ [10%]

(c) (i) The work function of the metal is larger than that of the n-type Si, hence a built-in potential forms that drops across the oxide, but a proportion will be taken up in band bending in the Si, and this will induce a depletion at the Si/oxide interface



(c)(ii) $V_T = -\dfrac{Q_d}{C_i} - 2V_f + \dfrac{\Phi_M - \Phi_{SC}}{e}$ [15%]

where $C_i$ is the oxide capacitance per unit area, $Q_d$ is the charge per unit area in the depletion region at strong inversion $Q_d = eN_D w_{max} = 2\left(\varepsilon_0\varepsilon_r eN_D V_f\right)^{1/2}$ and $eV_f$ is the difference between $E_{Fn}$ and $E_{Fi}$
(as defined in 3B5 lecture notes). [15%]

## Question 4

(a) For the one-sided p-n junction the depletion region may be considered to be basically entirely in the (lower doped) n-type region. The Poisson equation states

$$\nabla^2 V = \dfrac{-\rho}{\varepsilon_0\varepsilon_r} = \dfrac{-eN_D}{\varepsilon_0\varepsilon_r}$$

This assumes abrupt junction model, and donors to be fully ionised.

Given that V only varies in the x direction across the junction this becomes

$$\varepsilon_0\varepsilon_r \dfrac{d^2V}{dx^2} = -eN_D$$

Assuming that there are no electric fields outside the depletion region, i.e. the E-field is 0 at x=w (whereby w is the width of the depletion region), integration gives

$$-E = \dfrac{dV}{dx} = \dfrac{eN_D}{\varepsilon_0\varepsilon_r}(w - x)$$

Integration again with the boundary condition that V=0 at x=0 gives

$$V = \frac{eN_D}{\varepsilon_0 \varepsilon_r}\left(wx - \frac{x^2}{2}\right)$$

which may be evaluated at x=w to give the contact potential

$$V_0 = \frac{eN_D w^2}{2\varepsilon_0 \varepsilon_r}$$

Rearranging gives

$$w = \left(\frac{2\varepsilon_0 \varepsilon_r V_0}{eN_D}\right)^{1/2}$$
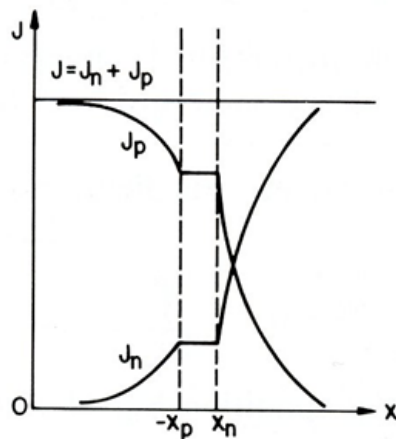[30%]

(b) Junction capacitance $C_d = \dfrac{dQ}{dV} = \dfrac{\varepsilon_0 \varepsilon_r}{w}$

For $C_d$ to double, $w$ needs to half. Hence forward bias $V_a$ is required (positive terminal connected to p-side)

$$w = \left(\frac{2\varepsilon_0 \varepsilon_r (V_0 - V_a)}{eN_D}\right)^{\frac{1}{2}}$$

Hence for w to half, $V_a = \dfrac{3}{4}V_0$
[20%]

(c)



[15%]

(d)

**GaAs**

**GaAlAs**

$E_{VAC}$

$E_C$

large barrier to electron injection

$p^+$

$n$

$E_V$
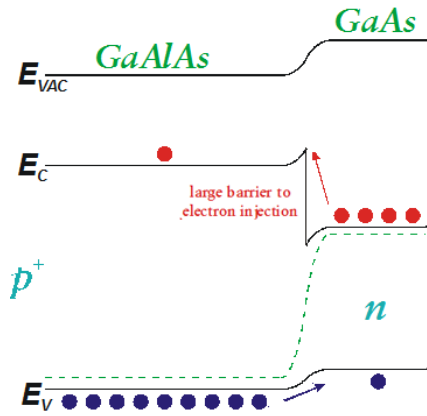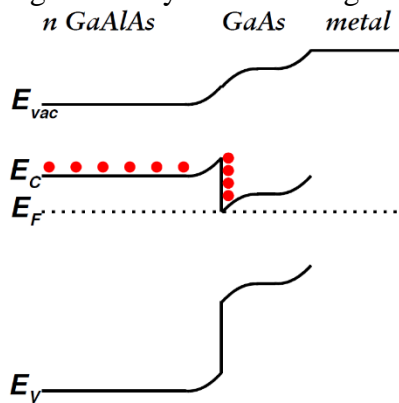
[15%]

(e) A so-called high electron mobility transistor (HEMT) uses as channel a wide bandgap doped semiconductor (here the AlGaAs) with a thin, intrinsic/low doped semiconductor (here GaAs). The electron mobility of GaAs is much higher than its hole mobility, so the AlGaAs would be n-doped to form a heterojunction with an accumulation of electrons in the GaAs layer. This allows a MESFET channel that has high mobility as well as high carrier density.



*n GaAlAs*    *GaAs*    *metal*

$E_{vac}$

$E_C$

$E_F$

$E_v$

[20%]