Electrons in Solids
(2012)

Classwork 1

(corrected – version 2)

The 2–dimensional free electron model (2D FEM) has a time independent Schrödinger equation (TISE) of the form:

$$-\frac{\hbar^2}{2m}\left(\frac{d^2\psi}{dx^2}+\frac{d^2\psi}{dy^2}\right)=E\psi$$

The solid consists of a square in the x-y plane with sides of equal length L.

1) What are the 2-dimensional Born von Karman boundary conditions?

2) Show that the TISE has solutions of the form:

$$\psi(x,y)=C\exp(i(k_x x+k_y y))$$

   Find the dispersion relationship and the possible values of k_x and k_y.

3) Normalize the solution to find the value of C.

4) Find the area in k-space per state.

5) By considering the number of states dn which lie between k and $k+dk$ in the k_x-k_y plane in k-space, show that the 2D FEM DOS is:

$$D(E)=\frac{mL^2}{\pi\hbar^2}$$

***(Original answer to 5) was out by factor of ½ - now corrected)*

Electrons in Solids
(2012)

Classwork 2

Magnesium (Mg) belongs to Group 2A (valency of 2) and has a density of $1.74\text{x}10^3$ kg m^{-3} and an atomic weight of $24.3\text{x}10^{-3}$ kg mol^{-1}. Consider the 3–dimensional free electron model (3D FEM).

1) Calculate the electron density N/V (in m^{-3}) for Mg.

2) By considering the volume in k-space occupied by N electrons and the volume in k-space per state, find the general equation for the Fermi wavevector k_F. Calculate its value for Mg (in m^{-1}).

3) Calculate the value of the Fermi velocity v_F of Mg in units of c.

4) If the electron mobility is 0.01 m^2 V^{-1} s^{-1}, under an applied electric field of 10^6 V m^{-1} calculate the drift velocity v_{drift} (in m s^{-1}). Hence, find the fraction δk by which the Fermi sphere has shifted in k-space under this applied electric field in units of k_F.

5) From the answer to 2), find the general equation for the Fermi energy E_F. Calculate its value for Mg (in eV).

6) By considering the rate of change of N with E_F, find the 3D FEM DOS.

7) Calculate the Fermi temperature T_F (in K) for Mg. From this calculate the ratio of k_BT/E_F at 300K.

8) Find the electron density n_{kT}/V in the energy range E_F to E_F+k_BT.

9) Calculate the fraction of total electrons in the energy range E_F to E_F+k_BT.

10) At low temperatures the mass specific heat capacity at constant volume c_V (in J kg^{-1} K^{-1}) of Mg is observed to follow:

$$c_V \approx \gamma T$$

Using the 3D FEM, calculate the value of γ for Mg. Compare this to the experimentally measured value of 0.07 J kg^{-1} K^{-2}. At 10K, how does the 3D FEM and experimentally measured values of c_V compare to that predicted by classical free electron gas theory?

Electrons in Solids
(2012)

Classwork 3

A 3-dimensional Bloch wavefunction has the form:

$$\psi(\boldsymbol{r}) = u_k(\boldsymbol{r}).\exp(i\boldsymbol{k}.\boldsymbol{r})$$

where: $$u_k(\boldsymbol{r}+\boldsymbol{R}) = u_k(\boldsymbol{r})$$

for all $\boldsymbol{R}$ in the crystal lattice, where:

$$\boldsymbol{R} = ua\hat{\boldsymbol{x}} + va\hat{\boldsymbol{y}} + wa\hat{\boldsymbol{z}}$$

for all integer values of u, v and w, and where a is the unit cell length. Let the solid have cubic shape with equal sides L.

1) Show that translation of the Bloch electron between unit cells results in a phase shift ϕ, and find its relationship to $\boldsymbol{k}$.

2) Show that the probability of the Bloch electron being found in any unit cell in the crystal structure is the same.

3) Find the 3-dimensional Born von Karman boundary conditions in the form of $\psi(\boldsymbol{r}+\boldsymbol{R})$.

4) Hence, find the allowed values of quantum number $\boldsymbol{k}$.

5) At small $\boldsymbol{k}$ and small U_0, where U_0 is related to the magnitude of the periodic potential, the dispersion relationship can be approximated by:

$$E = \left(\frac{6U_0}{U_0+3}\right)\frac{\hbar^2}{2ma^2} + \left(\frac{3}{U_0+3}\right)\frac{\hbar^2|\boldsymbol{k}|^2}{2m}$$

Find the density of states.

Electrons in Solids
(2012)

Classwork 4

Consider the Bloch wavefunction:

$$\psi_{k'}(x) = u_{k'}(x)\exp(ik'x)$$

where *k'* is in the 4th Brillouin Zone in the $+k_x$ direction. This wavevector value can be translated into the 1st Brillouin zone using:

$$k' = k + \frac{2\pi}{a}n'$$

where *n'* is an integer.

1) What is the value of *n'*?
2) Show that this Bloch wavefunction can be translated into the 1st Brillouin zone to form a new Bloch wavefunction with this wavevector *k*.

Bloch electrons have group velocity v_g. If a force *F* acts on the Bloch electron it accelerates:

$$F = m^* \frac{dv_g}{dt}$$

where m^* is the effective mass. Assume that *F*, v_g and *k* are in the *x* direction.

3) Find an equation relating the group velocity v_g to *E* and *k*.
4) By considering the work done δE by a force *F* in time δt, show that:

$$\frac{dk}{dt} = \frac{F}{\hbar}$$

5) Hence, find an equation relating the effective mass m^* to *E* and *k*.

Consider a semiconductor in which the conduction band dispersion curve $E_C(k)$ and the valence band dispersion curve $E_V(k)$ close to $k = 0$ in the reduced zone scheme can be described by:

$$E_C(k) = 7.56\times10^{-38}k^2 + 4.02\times10^{-19}$$
$$E_V(k) = -1.48\times10^{-38}k^2$$

where E_V and E_C are in Joules and the magnitude of the electron wavevector *k* is in m^{-1}.

6) What is the energy gap E_G (in eV)?
7) What is the effective mass of an electron m_n^* in the conduction band (in units of the free electron rest mass m_e)?
8) What is the effective mass of an electron m_n^* in the valence band (in units of m_e)?
9) What is the effective mass of a hole m_p^* in the valence band (in units of m_e)?

Electrons in Solids
(2012)

Classwork 1
SOLUTIONS

(corrected – version 2)

1) What are the 2-dimensional Born von Karman boundary conditions?

$$\psi(x,y) = \psi(x+L,y)$$
$$\psi(x,y) = \psi(x,y+L)$$

1) Show that the TISE has solutions of the form:

$$\psi(x,y) = C\exp(i(k_x x + k_y y))$$

Find the dispersion relationship and the possible values of k_x and k_y.

Rearrange TISE:

$$\left(\frac{d^2\psi}{dx^2} + \frac{d^2\psi}{dy^2}\right) = -\frac{2mE}{\hbar^2}\psi$$

Trial solution:

$$\psi(x,y) = C\exp(i(k_x x + k_y y))$$
$$= C\exp(ik_x x)\exp(ik_y y)$$
$$= CX(x)Y(y)$$

Solve:

$$C\left(Y\frac{d^2X}{dx^2} + X\frac{d^2Y}{dy^2}\right) = -\frac{2mE}{\hbar^2}CXY$$
$$\left(\frac{X''}{X} + \frac{Y''}{Y}\right) = -\frac{2mE}{\hbar^2}$$

Leads to:

$$\left(k_x^2 + k_y^2\right) = \frac{2mE}{\hbar^2}$$
$$E = \frac{\hbar^2|\underline{\boldsymbol{k}}|^2}{2m}$$
$$\underline{\boldsymbol{k}} = (k_x, k_y)$$

For k values:

$$\psi(x,y) = \psi(x+L,y)$$
$$\psi(0,0) = \psi(0+L,0)$$
$$C = C\exp(ik_x L)$$
$$k_x L = 2\pi n_x$$
$$k_x = \frac{2\pi n_x}{L}$$
$$k_y = \frac{2\pi n_y}{L}$$

For n_x and n_y = 0, ±1, ±2, ±3, ±4,……

2) Normalize the solution to find the value of C.

$$\int_0^L \int_0^L \psi(x,y).\psi^*(x,y)dxdy = 1$$
$$= \int_0^L \int_0^L C^2 dxdy$$
$$= C^2 L^2 = 1$$
$$C = \frac{1}{L}$$

$$\psi(x,y) = \frac{1}{L}\exp(ik_x x)\exp(ik_y y)$$

3) Find the area in k-space per state.

$$k_x = \frac{2\pi n_x}{L}$$
$$\Delta k_x = k_x(n_x = 1) = \frac{2\pi}{L}$$
$$\Delta k_y = k_y(n_y = 1) = \frac{2\pi}{L}$$
$$\Delta k_x \Delta k_y = \left(\frac{2\pi}{L}\right)^2$$

4) By considering the number of states *dn* which lie between *k* and *k+dk* in the k_x-k_y plane in *k*-space, show that the 2D FEM DOS is:

$$D(E) = \frac{mL^2}{\pi\hbar^2}$$

***(Original answer was out by factor of ½ - now corrected)*

States *dn* in area occupied in k-space between *k* & *k+dk:*

$$n = |\boldsymbol{n}|$$
$$k = |\boldsymbol{k}|$$
$$\Delta k_x \Delta k_y dn = 2\pi k dk$$
$$\frac{dn}{dk} = \frac{2\pi k}{\Delta k_x \Delta k_y} = \frac{L^2}{2\pi} k$$
$$k = \frac{\sqrt{2m}}{\hbar}\sqrt{E}$$
$$\frac{dk}{dE} = \frac{\sqrt{2m}}{2\hbar}\frac{1}{\sqrt{E}}$$
$$\frac{dn}{dk} = \frac{L^2}{2\pi}\frac{\sqrt{2m}}{\hbar}\sqrt{E}$$
$$\frac{dn}{dk}\frac{dk}{dE} = \frac{dn}{dE} = \frac{L^2}{2\pi}\frac{2m}{2\hbar^2} = \frac{mL^2}{2\pi\hbar^2}$$
$$Spin : \times 2$$
$$D(E) = \frac{mL^2}{\pi\hbar^2}$$

***(Mistake in original – wrote circumference of circle in k-space as πk - now corrected to 2πk)*
***(Original answer was out by factor of ½ - now corrected)*

Electrons in Solids
(2012)

Classwork 2
SOLUTIONS

Magnesium (Mg) belongs to Group 2A (valency of 2) and has a density of 1.74×10^{3} kg m^{-3} and an atomic weight of 24.3×10^{-3} kg mol^{-1}. Consider the 3–dimensional free electron model (3D FEM).

1) Calculate the electron density N/V (in m^{-3}) for Mg.

   Atomic density = $(\rho/A).N_A = 4.29 \times 10^{28}$ m^{-3}
   Valence electron density = $2.(\rho/A).N_A = 8.6 \times 10^{28}$ m^{-3}

2) By considering the volume in k-space occupied by N electrons and the volume in k-space per state, find the general equation for the Fermi wavevector k_F. Calculate its value for Mg (in m^{-1}).

   Volume of free electron sphere containing N electrons:

   $$\frac{4}{3}\pi k_F^3$$

   Volume per state in k-space:

   $$\Delta k_x \Delta k_y \Delta k_z = \left(\frac{2\pi}{L}\right)^3$$

   Therefore, with 2 electrons per state:

   $$\frac{N}{2} = \frac{4}{3}\pi k_F^3 \left(\frac{L}{2\pi}\right)^3$$

   $$N = \frac{8}{3}\pi k_F^3 \frac{V}{8\pi^3}$$

   $$\frac{N}{V} = \frac{1}{3}k_F^3 \frac{1}{\pi^2}$$

   $$k_F = \left(3\pi^2 \frac{N}{V}\right)^{1/3}$$

   Therefore $k_F = 1.36 \times 10^{10}$ m^{-1}

3) Calculate the value of the Fermi velocity v_F of Mg in units of c.

   $v_F = \hbar k_F/m = 1.57 \times 10^{6}$ m/s $= 0.0052c \approx 0.5\%c$

4) If the electron mobility is 0.01 m^2 V^{-1} s^{-1}, under an applied electric field of 10^6 V m^{-1} calculate the drift velocity v_{drift} (in m s^{-1}). Hence, find the fraction δk by which the Fermi sphere has shifted in k-space under this applied electric field in units of k_F.

$v_{drift} = \mu_n E_{field} = 10^4$ m/s
$\delta k = (v_{drift}/v_F)k_F = 0.0064k_F$

5) From the answer to 2), find the general equation for the Fermi energy E_F. Calculate its value for Mg (in eV).

$$k_F = \left(3\pi^2 \frac{N}{V}\right)^{1/3}$$

$$E_F = \frac{\hbar^2 k_F^2}{2m}$$

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

$E_F = (\hbar k_F)^2/2m = m(v_F)^2/2 = 1.12\text{x}10^{-18}$ J = 7.02 eV

6) By considering the rate of change of N with E_F, find the 3D FEM DOS.

Non-formal method to find $D(E)$: we assume rate of change of N with E_F same as rate of change of n with E

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

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

$$\frac{dN}{dE_F} = \frac{dn}{dE} = D(E) = \frac{V}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\sqrt{E_F}$$

7) Calculate the Fermi temperature T_F (in K) for Mg. From this calculate the ratio of k_BT/E_F at 300K.

$T_F = E_F/k_B = 81{,}200$ K
$300k_B/E_F = 300/T_F = 0.0037$

8) Find the electron density n_{kT}/V in the energy range E_F to E_F+k_BT.

$D(E_F)$ = 1.14x10^{47} m^{-3} J^{-1}
$n_{kT}/V = D(E_F).k_BT$ = 4.72x10^{26} m^{-3}

9) Calculate the fraction of total electrons in the energy range E_F to E_F+k_BT.

$(n_{kT}/V)/(N/V)$ = 0.0055

10) At low temperatures the mass specific heat capacity at constant volume c_V (in J kg^{-1} K^{-1}) of Mg is observed to follow:

$$c_V \approx \gamma T$$

Using the 3D FEM, calculate the value of γ for Mg. Compare this to the experimentally measured value of 0.07 J kg^{-1} K^{-2}. At 10K, how does the 3D FEM and experimentally measured values of c_V compare to that predicted by classical free electron gas theory?

3D FEM

$C_v/T = 3(N/V)(k_B)^2/E_F$ = 43.9 J m^{-3} K^{-2}

$c_v/T = C_v/T\rho$ = 0.025 J kg^{-1} K^{-2}

Classical

$C_v = (N/V)(k_B)$ = 1.2x10^6 J m^{-3} K^{-1}

$c_v = C_v/\rho$ = 682 J kg^{-1} K^{-1}

At 10K:
3D FEM c_v = 0.25 J kg^{-1} K^{-1}
measured c_v = 0.7 J kg^{-1} K^{-1}
classical c_v = 682 J kg^{-1} K^{-1}

Classical out by 3 orders of magnitude and cannot explain T dependence.

Electrons in Solids
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Classwork 3
SOLUTIONS

A 3-dimensional Bloch wavefunction has the form:

$$\psi(\boldsymbol{r}) = u_k(\boldsymbol{r}).\exp(i\boldsymbol{k}.\boldsymbol{r})$$

where: $$u_k(\boldsymbol{r}+\boldsymbol{R}) = u_k(\boldsymbol{r})$$

for all $\boldsymbol{R}$ in the crystal lattice, where:

$$\boldsymbol{R} = ua\hat{\boldsymbol{x}} + va\hat{\boldsymbol{y}} + wa\hat{\boldsymbol{z}}$$

for all integer values of u, v and w, and a is the unit cell length. Let the solid have cubic shape with equal sides L.

1) Show that translation of the Bloch electron between units cells results in a phase shift ϕ, and find its relationship to $\boldsymbol{k}$.

$$\psi(\boldsymbol{r}+\boldsymbol{R}) = u_k(\boldsymbol{r}+\boldsymbol{R})\exp(i\boldsymbol{k}.(\boldsymbol{r}+\boldsymbol{R}))$$
$$= u_k(\boldsymbol{r})\exp(i\boldsymbol{k}.\boldsymbol{r})\exp(i\boldsymbol{k}.\boldsymbol{R})$$
$$= \psi(\boldsymbol{r})\exp(i\boldsymbol{k}.\boldsymbol{R})$$
$$\exp(i\phi) = \exp(i\boldsymbol{k}.\boldsymbol{R})$$
$$\phi = \boldsymbol{k}.\boldsymbol{R}$$

2) Show that the probability of the Bloch electron being found in any unit cell in the crystal structure is the same.

$$\psi(\boldsymbol{r}+\boldsymbol{R}) = \psi(\boldsymbol{r})\exp(i\boldsymbol{k}.\boldsymbol{R})$$

$$\psi^*(\boldsymbol{r}+\boldsymbol{R}).\psi(\boldsymbol{r}+\boldsymbol{R})$$
$$= \psi^*(\boldsymbol{r})\exp(-i\boldsymbol{k}.\boldsymbol{R}).\psi(\boldsymbol{r})\exp(i\boldsymbol{k}.\boldsymbol{R})$$
$$= \psi^*(\boldsymbol{r}).\psi(\boldsymbol{r})$$

$$\therefore \left|\psi^*(\boldsymbol{r}+\boldsymbol{R}).\psi(\boldsymbol{r}+\boldsymbol{R})\right| = \left|\psi^*(\boldsymbol{r}).\psi(\boldsymbol{r})\right|$$

3) Find the 3-dimensional Born von Karman boundary conditions in the form of $\psi(\boldsymbol{r}+\boldsymbol{R})$.

$$\psi(x,y,z)=\psi(x+L,y,z)$$
$$\psi(x,y,z)=\psi(x,y+L,z)$$
$$\psi(x,y,z)=\psi(x,y,z+L)$$

$$\psi(\boldsymbol{r})=\psi(\boldsymbol{r}+\boldsymbol{R})$$
$$\boldsymbol{R}=L\hat{\boldsymbol{x}}+L\hat{\boldsymbol{y}}+L\hat{\boldsymbol{z}}$$

4) Hence, find the allowed values of quantum number $\boldsymbol{k}$.

$$\psi(\boldsymbol{r}+\boldsymbol{R})=\psi(\boldsymbol{r})\exp(i\boldsymbol{k}.\boldsymbol{R})$$
$$=\psi(\boldsymbol{r})\exp(ik_x.L)\exp(ik_y.L)\exp(ik_z.L)$$
$$1=\exp(ik_x.L)\exp(ik_y.L)\exp(ik_z.L)$$
$$k_x=\frac{2\pi}{L}n_x$$
$$k_y=\frac{2\pi}{L}n_y$$
$$k_z=\frac{2\pi}{L}n_z$$
$$L=Na$$
$$n_x,n_y,n_z=0,\pm1,\pm2,\pm3,...$$
$$\boldsymbol{k}=(k_x,k_y,k_z)$$

5) At small $\boldsymbol{k}$ and small U_0, where U_0 is related to the magnitude of the periodic potential, the dispersion relationship can be approximated by:

$$E=\left(\frac{6U_0}{U_0+3}\right)\frac{\hbar^2}{2ma^2}+\left(\frac{3}{U_0+3}\right)\frac{\hbar^2|\boldsymbol{k}|^2}{2m}$$

Find the density of states.

$$\Delta k_x \Delta k_y \Delta k_z = \left(\frac{2\pi}{L}\right)^3$$

$$\frac{dn}{dk} = \left(\frac{2\pi}{L}\right)^{-3} 4\pi k^2$$

$$E = \left(\frac{6U_0}{U_0+3}\right)\frac{\hbar^2}{2ma^2} + \left(\frac{3}{U_0+3}\right)\frac{\hbar^2|\boldsymbol{k}|^2}{2m} = A + B|\boldsymbol{k}|^2$$

$$k = |\boldsymbol{k}| = \sqrt{\frac{E-A}{B}}$$

$$\frac{dk}{dE} = \frac{1}{2B}\left(\frac{E-A}{B}\right)^{-1/2}$$

$$\frac{dn}{dk}.\frac{dk}{dE} = \left(\frac{2\pi}{L}\right)^{-3} 4\pi k^2 \frac{1}{2B}\left(\frac{E-A}{B}\right)^{-1/2} = \left(\frac{2\pi}{L}\right)^{-3} 4\pi \frac{1}{2B}\left(\frac{E-A}{B}\right)^{1/2}$$

$$D(E) = 2\frac{dn}{dk}.\frac{dk}{dE} = \frac{V}{4\pi^2}\left(\frac{E-A}{B^3}\right)^{1/2}$$

Electrons in Solids
(2012)

Classwork 4
SOLUTIONS

Consider the Bloch wavefunction:

$$\psi_{k'}(x) = u_{k'}(x)\exp(ik'x)$$

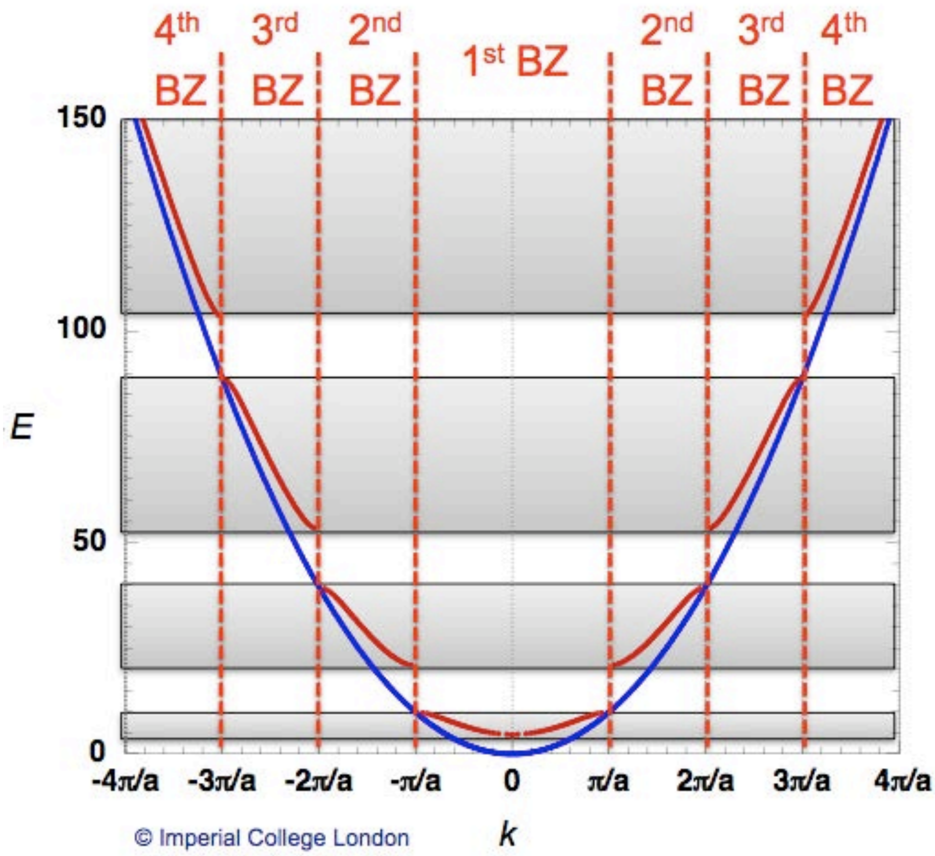
where *k'* is in the 4th Brillouin Zone in the $+k_x$ direction. This wavevector value can be translated into the 1st Brillouin zone using:

$$k' = k + \frac{2\pi}{a}n'$$

where *n'* is an integer.

1) What is the value of *n'*?

BZ structured as below (see Lecture 13).



To reach 4th BZ (in +x direction) from 1st BZ (in units of 2π/a) requires a shift of 2x2π/a = 4π/a. Hence n' = 2.

2) Show that this Bloch wavefunction from can be translated into the 1st Brillouin zone to form a new Bloch wavefunction with wavevector *k*.

$$\psi_{k'}(x) = u_{k'}(x)\exp(ik'x)$$
$$k' = k + \frac{2\pi}{a}n'$$
$$\psi_{k'}(x) = u_{k'}(x)\exp(ikx)\exp(i\frac{2\pi}{a}n')$$
$$= \left[u_{k'}(x)\exp(i\frac{2\pi}{a}n')\right]\exp(ikx)$$

Define:

$$u_k(x) = u_{k'}(x)\exp(i\frac{2\pi}{a}n'x)$$

Is of Bloch form:

$$u_k(x+na) = u_{k'}(x+na)\exp(i\frac{2\pi}{a}n'x)\exp(i\frac{2\pi}{a}n'.na)$$
$$= u_{k'}(x)\exp(i\frac{2\pi}{a}n'x) = u_k(x)$$

Therefore can write:

$$\psi_{k'}(x) = u_{k'}(x)\exp(ik'.x)$$
$$= \left(u_{k'}(x)\exp(i\frac{2\pi}{a}x)\right)\exp(ik.x)$$
$$= u_k(x)\exp(ik.x)$$
$$= \psi_k(x)$$

Bloch electrons have group velocity v_g. If a force F acts on the Bloch electron it accelerates:

$$F = m^* \frac{dv_g}{dt}$$

where m^* is the effective mass. Assume that F, v_g and k are in the x direction.

3) Find an equation relating the group velocity v_g to E and k.

$$v_g = \frac{d\omega}{dk}$$
$$E = \hbar\omega$$
$$\therefore v_g = \frac{1}{\hbar}\frac{dE}{dk}$$

4) By considering the work done δE by a force F in time δt, show that:

$$\frac{dk}{dt} = \frac{F}{\hbar}$$

$$\delta E = F.(v_g \delta t)$$
$$\frac{\delta E}{\delta t} = F v_g$$
$$\frac{\delta E}{\delta t} = \frac{dE}{dt} = \frac{dE}{dt}\frac{dk}{dk} = \frac{dE}{dk}\frac{dk}{dt} = F v_g$$
$$v_g = \frac{1}{\hbar}\frac{dE}{dk}$$
$$\frac{dE}{dk}\frac{dk}{dt} = F\frac{1}{\hbar}\frac{dE}{dk}$$
$$\therefore \frac{dk}{dt} = \frac{F}{\hbar}$$

5) Hence, find an equation relating the effective mass m^* to E and k.

$$v_g = \frac{1}{\hbar}\frac{dE}{dk}$$
$$\frac{dv_g}{dt} = \frac{1}{\hbar}\frac{d^2E}{dkdt}$$
$$= \frac{1}{\hbar}\left(\frac{d^2E}{dk^2}\right)\frac{dk}{dt} = \frac{1}{\hbar}\left(\frac{d^2E}{dk^2}\right)\frac{F}{\hbar}$$
$$F = \hbar^2\left(\frac{d^2E}{dk^2}\right)\frac{dv_g}{dt}$$
$$m^* = \hbar^2\left(\frac{d^2E}{dk^2}\right)^{-1}$$

In a semiconductor, the conduction band dispersion curve $E_C(k)$ and the valence band dispersion curve $E_V(k)$ close to $k = 0$ in the reduced zone scheme can be described by:

$$E_C(k) = 7.56 \times 10^{-38} k^2 + 4.02 \times 10^{-19}$$
$$E_V(k) = -1.48 \times 10^{-38} k^2$$

where E_V and E_C are in Joules and the magnitude of the electron wavevector k is in m^{-1}.

6) What is the energy gap E_G (in eV)?

Calculate in centre of 1st BZ at k = 0

$$E_C(0) = 4.02 \times 10^{-19}$$
$$E_V(0) = 0$$
$$E_G = E_C - E_V$$
$$= 4.02 \times 10^{-19} J$$
$$= 2.50 eV$$

7) What is the effective mass of an electron m_n* in the conduction band (in units of the free electron rest mass m_e)?

$$\frac{\partial^2 E_C(k)}{\partial k^2} = 2 \times 7.56 \times 10^{-38} = 15.1 \times 10^{-38}$$
$$m_n^* = \hbar^2 \left(\frac{d^2E}{dk^2} \right)^{-1} = \frac{\left(1.05 \times 10^{-34}\right)^2}{15.1 \times 10^{-38}}$$
$$= 0.73 \times 10^{-31} kg = 0.08 m_e$$

8) What is the effective mass of an electron m_n* in the valence band (in units of m_e)?

$$\frac{\partial^2 E_C(k)}{\partial k^2} = 2 \times -1.48 \times 10^{-38} = -2.96 \times 10^{-38}$$
$$m_n^* = \hbar^2 \left(\frac{d^2E}{dk^2} \right)^{-1} = \frac{\left(1.05 \times 10^{-34}\right)^2}{-2.96 \times 10^{-38}}$$
$$= -3.72 \times 10^{-31} kg = -0.41 m_e$$

9) What is the effective mass of a hole m_p* in the valence band (in units of m_e)?

$$m_p^* = -m_n^* = 0.41 m_e$$