Condensed Matter Physics 3
Example Workshop 2 – Solution

1. Properties of electrons in Bloch energy bands.

(a) The effective mass is given by

$$m_{eff} = \hbar^2 \left(\frac{d^2E}{dk^2} \right)^{-1}$$

[This is the inverse curvature of the energy band].

(b) To determine the effective mass we need to evaluate:

$$\frac{d^2E}{dk^2} = -Aa^2 \cos(ka)$$

At $k = 0$, $\quad m_{eff} = \dfrac{-\hbar^2}{Aa^2 \cos(0)} = \dfrac{-\hbar^2}{Aa^2}$

At $k = \pi/a$ $\quad m_{eff} = \dfrac{+\hbar^2}{Aa^2 \cos(\pi)} = \dfrac{+\hbar^2}{Aa^2}$.

[Note the change in sign from centre and edge of Brillouin zone. This is due to the opposite curvature of the energy bands.]

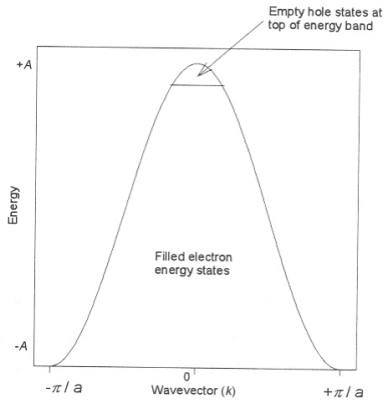
(c) The group velocity of the electrons is given by $v_g = \dfrac{1}{\hbar}\left(\dfrac{dE}{dk} \right)$. From the *E*-*k* relation given, this is equal to 0 at both $k = 0$ and $k = \pi/a$.

(*d*) The total current carried by a completely full band is zero. (The average velocity distribution is zero, and this does not change under applied electric field – there are no empty electron states to move into so the average velocity distribution is still zero). The current carried by the nearly full band is then equal to the current carried by full band-current that would be carried by missing states = $0 - (-e)n_h v = +en_h v$.

(*e*) This is the same as a current that would be carried by n_h holes (of charge $+e$) per unit length moving with a velocity *v*.

(*f*) The diagram shows a sketch of the energy band from $k = -\pi/a$ to $+\pi/a$.

The vacant states at the top of the energy band can be thought of as full with positively charged holes.



2. Properties of electrons in Bloch energy bands.

(*a*) In one-dimensional free electron theory the allowed electron energy states are distributed over all energies

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

The free electron wavefunctions are then of the form $\psi_k(x) = exp(ikx)$ and they represent running (travelling) waves and carry momentum $p = \hbar k$. Consider a one-dimensional solid composed of a chain of atoms of lattice constant *a*. The Bragg condition $(k + \mathrm{G})^2 = k^2$ for diffraction of a wave of wavevector *k* then becomes (in one-dimension)

$$k = \pm\frac{1}{2}\mathrm{G} = \pm n\,\pi/a$$

where G = 2*nπ*/*a* is a reciprocal lattice vector and *n* is an integer.
The first reflections and the first energy gap occur at $k = \pm\pi/a$. The region in *k*-space between -*π*/*a* and +*π*/*a* is the first Brillouin zone of the lattice. Other energy gaps occur for other values of the integer *n*.

(*b*) The wavefunctions at $k = \pm\pi/a$ are not the travelling waves of the form exp(*iπx*/*a*) or exp(-*iπx*/*a*) of free electrons we might expect. At these special values of *k* the wavefunctions are made up of equal parts of waves travelling to the right and waves travelling to the left. When the Bragg reflection condition $k = \pm\pi/a$ is satisfied by the wavevector, a wave travelling to the right is Bragg-reflected so as to travel to the left, and vice versa. Each subsequent Bragg reflection reverses the direction of travel of the wave. The time-independent result is a standing wave.

We can form two different standing waves from the two travelling waves $\exp(i\pi x/a)$, namely

$$\psi(+) = \exp(i\pi x/a) + \exp(-i\pi x/a) = 2\cos(\pi x/a)$$

$$\psi(-) = \exp(i\pi x/a) - \exp(-i\pi x/a) = 2i\,\sin(\pi x/a)$$

The standing waves are labelled (+) or (-) according to whether or not they change sign when –*x* is substituted for *x*. Both standing waves are composed of equal parts of right- and left-directed traveling waves.

(*c*) The two standing waves *ψ*(+) and *ψ*(-) pile up electron density in different regions and therefore have different potential energies. The probability density *ρ* of a particle is $\psi^*\psi = |\psi|^2$. For the standing wave *ψ*(+) we have $\rho(+) = |\psi|^2 \propto cos^2\pi\,x/a$. For the other standing wave *ψ*(-) the probability density is $\rho(-) = |\psi|^2 \propto \sin^2\pi\,x/a$, which concentrates electron density between the positive ion cores.

The wavefunctions at the Brillouin zone boundary $k = \pi/a$ are $\sqrt{\frac{2}{a}}\cos\pi x/a$ and $\sqrt{\frac{2}{a}}\sin\pi x/a$, normalised over unit length of line. Let us suppose that the potential energy of an electron in the one-dimensional crystal at point *x* is $U(x) = U\cos 2\pi x/a$
The first-order energy difference between the two standing waves is

$$E_g = \int_0^a dx\; U(x)\;[|\psi(+)|^2 - |\psi(-)|^2]$$

$$= \frac{2}{a}\int_0^a U\;\cos(2\pi x/a)\,(\cos^2\pi x/a - \sin^2\pi x/a)dx = U$$

Thus, the energy gap is equal to the Fourier component of the crystal potential.

(*d*) We know for ordinary travelling waves that the group velocity is given by

$$v_{\text{group}} = \frac{d\omega}{dk}$$

As $E = \hbar\omega$ then it follows that

$$v_{\text{group}} = \frac{1}{\hbar}\frac{dE(k)}{dk}$$

For an electron at the bottom of an energy band in the nearly-free electron model $E = \frac{\hbar^2 k^2}{2m^*}$ so

$$v_{\text{group}} = \frac{1}{\hbar}\frac{d}{dk}\left[\frac{\hbar^2 k^2}{2m^*}\right] = \frac{\hbar k}{m^*} = \frac{p}{m^*} = v$$

Where *p* is the crystal momentum of the Bloch electrons.

Once we know the velocity of an electron in a band we can determine the current carried by a collection of electrons in an energy band. The current density is given by $j = ne\langle v\rangle$ where $\langle v\rangle$ is the average velocity of electrons in the band. Suppose we have M energy states in an energy band occupied by $2M$ electrons. We then have

$$\langle v\rangle = \frac{a}{\hbar}\int_{k=-\pi/a}^{k=\pi/a}\frac{dE}{dk}\frac{dk}{2\pi}$$

or,

$$\langle v\rangle = \frac{a}{2\pi\hbar}[E(\pi/a) - E(-\pi/a)]$$

As we found earlier $k = \pm\pi/a$ are physically equivalent values of the Bloch wavevector. So $E(\pi/a) = E(-\pi/a)$ and $\langle v\rangle = 0$. If $\langle v\rangle = 0$ then $j = 0$ and the total current carried by the energy band is zero. This is an important result: a completely filled energy band makes no contribution to the current carried by a crystal.