Effective Mass

a) For a free electron: $\varepsilon = KE = \frac{1}{2}mv^2 = p^2/2m$ (since $\mathbf{p} = m\mathbf{v}$);

in quantum theory, $p_x = \int\psi^* p_{op}\,\psi\, dx$; $\psi_{free\ e} = Ae^{ikx}$; $p_{op} = -i\hbar\,\partial/\partial x$;

therefore for free electron:

$p_x = \int(Ae^{-ikx})(-i\hbar\partial[Ae^{ikx}]/\partial x)\,dx = \hbar k\int A^2dx = \hbar k(1) = \hbar k_x$, or $\mathbf{p} = \hbar\mathbf{k}$.

Note that Probability = $\int\psi^*\psi dx = \int A^2 dx = 1$ since the sum of probabilities must total one.

Now note: $\varepsilon = p^2/2m = \hbar^2k^2/2m$; therefore $\partial\varepsilon/\partial k = 2\hbar^2k/2m = \hbar^2k/m$

and $\partial^2\varepsilon/\partial k^2 = \partial(\hbar^2k/m)/\partial k = \hbar^2/m$, or $\mathbf{m = \hbar^2/(\partial^2\varepsilon/\partial k^2)}$.

b) For electron in a periodic potential near the zone boundary:

recall: **at the zone boundary**, $k = \frac{1}{2}G$, we have: $\varepsilon(\pm) = \hbar^2(\frac{1}{2}G)^2/2m) \pm U$ so that $E_{gap} = 2|U|$

where $\varepsilon_{edge\text{-}free} = (\hbar^2(\frac{1}{2}G)^2/2m)$, and $\varepsilon_{edge} = \varepsilon(\pm) = \{\varepsilon_{edge\text{-}free} \pm U\}$,

and **near the zone boundary** with K' the amount of wavevector away from the zone boundary, we have,

with $k = \frac{1}{2}G + K'$, or $K' = k - \frac{1}{2}G$, see Part 3 Near Zone Boundary:

$\varepsilon_{conduction} = \varepsilon(-) + (\hbar^2K'^2/2m)(1 - 2\varepsilon_{edge}/U)$ (for U<0 this is higher band)

$\varepsilon_{valence} = \varepsilon(+) + (\hbar^2K'^2/2m)(1 + 2\varepsilon_{edge}/U)$ (for U<0 this is lower band).

We started, in Part 3 in the section on the Central Equation, with assuming our wavefunction was in series form (for now ignoring the time part, $T(t) = T_o e^{-i(\varepsilon/\hbar)t}$ which goes away when we take $\Psi^*\Psi$):

$\psi(x) = \Sigma_k C_k e^{ikx}$ where $k = n2\pi/L$, so the summation is really a sum over n;

if one particular k is chosen, however, then the sum is limited to a sum over the G's where $G_n = n2\pi/a$:

$\psi_k(\mathbf{r}) = \Sigma_G C_{k+G} e^{i(\mathbf{k}+\mathbf{G})\bullet\mathbf{r}}$ (essentially expressing ψ_k as a Fourier Series)

therefore $\mathbf{p} = \int(\Sigma_G C_{k+G} e^{-i(\mathbf{k}+\mathbf{G})\bullet\mathbf{r}})(-i\hbar\partial[\Sigma_G C_{k+G}) e^{i(\mathbf{k}+\mathbf{G})\bullet\mathbf{r}}]/\partial\mathbf{r}]dV$

$= \int\Sigma_G\, \hbar(\mathbf{k}+\mathbf{G})|C_{k+G}|^2dV = \hbar\mathbf{k}\int\Sigma_G|C_{k+G}|^2dV + \int\Sigma_G\,\hbar\mathbf{G}|C_{k+G}|^2dV$

and since $\int\Sigma_G|C_{k+G}|^2dV = 1$ (sum of the probabilities = 1) we have

$\mathbf{p} = \hbar\mathbf{k}$ + other = momentum of free electron + contribution due to the lattice

Now we **define effective mass**: $\mathbf{m^* \equiv \hbar^2/(d^2\varepsilon/dk^2)}$ (greater curvature implies smaller m*)

For an electron **in conduction band** near the zone boundary:

$m_e^* = \hbar^2/[d^2\varepsilon/dk^2] = \hbar^2/[d^2\{\varepsilon(-) + (\hbar^2K'^2/2m)(1 - 2\varepsilon_{edge}/U)\}/dk^2]$

so with $\varepsilon(-)$ = constant, and $K' = k - G/2$, taking the second derivative gives

$m_e^* = \hbar^2/[(\hbar^2/m_e)\{1 - 2\varepsilon_{edge}/U\}] = m_e/[1 - 2\varepsilon_{edge}/U]$

for U<0 and for $\varepsilon_{edge}/|U| \approx 10$, then $\mathbf{m_e^* \approx m_e/20}$!

For an electron **in valence band** near the zone boundary:

$m_e^* = \hbar^2/[d^2\varepsilon/dk^2] = \hbar^2/[d^2\{\varepsilon(+) + (\hbar^2K'^2/2m)(1 + 2\varepsilon_{edge}/U)\}/dk^2]$

$m_e^* = \hbar^2/[(h^2/m_e)\{1 + 2\varepsilon_{edge}/U\}] = m_e/[1 + 2\varepsilon_{edge}/U]$

for U<0 and for $\varepsilon_{edge}/|U| \approx 10$, then $m_e^* < 0$;

but since $m_{hole} = -m_e^*$, $\mathbf{m_{hole} > 0}$!

Physical basis for effective mass: reflection of an e from the lattice (and hence momentum transfer) depends on **k**; from ħ**k** = **p** = m**v**; KE = ½mv²; so KE = p²/(2m); KE and p^2 are related by 1/(2m) so that the smaller the mass, the bigger the coefficient relating p^2 and KE); this means that a small Δ**k** for a large ΔE acts like the electron has a very small mass; **a negative m^* means that on going from state k to k+δk, momentum transfer from electron to lattice is greater than from applied force to electron, which means that electron loses momentum as it gains energy – which acts like negative mass!** This happens for "missing" electron or hole in valence band.

The excel spreadsheet (in the last section of part 3), which was used to show the band gap and ε(k) near the zone boundary, can be modified to see the effect of different effective masses. Remember that the derivation of ε(k) near the zone boundary employed an approximation that removed most of the (smaller) coefficients, and so the actual ε(k) may be somewhat different than the derived ε(k). We take this into account by our definition of effective mass.

Homework Problem 31 *demonstrates effective mass and its relation to electron energies and momenta (and thus electron energies and wavevectors).*

c) Determining effective mass

One way of directly determining the effective mass of electrons in a semiconductor is by **cyclotron resonance**, which we now describe. If we place a magnetic field on the material, then the electrons will go in circles (until they collide and lose their orientation). As we will see below, the frequency of the orbit of the electrons is independent of their velocity, so all the electrons in the conduction band should orbit at the same frequency. If we apply electromagnetic energy of the same frequency as the orbiting electrons, they will be pushed forward when they are going forward on one side of the orbit and pulled back when they are going back on the other side of the orbit. This will effectively increase the energy of the electrons which means the electrons absorb the radiation. Thus by determining the frequency at which the electromagnetic radiation is absorbed, we determine the frequency the electrons are orbiting in the magnetic field. But that frequency depends on their effective mass:

$\Sigma \mathbf{F} = m^*\mathbf{a}$ where $\mathbf{F}_{mag} = q\mathbf{v}\times\mathbf{B}$, and $a_{circ} = \omega^2 r$ and $v_{circ} = \omega r$ so $a_{circ} = \omega v$

so $qvB = m^*\omega v$, or $\omega = qB/m^*$, or $\mathbf{m^* = m_{effective} = qB/\omega}$,

where q is the charge of the electron (q = -e), B is the applied magnetic field, and ω is the angular frequency (in radians/sec, f=ω/2π where f is in cycles/sec or Hz) of the incident (and absorbed) electromagnetic radiation.

Note: In order for the electrons to absorb the radiation, they must make at least a significant part of one orbit before they lose their orientation from scattering. Thus we need θ > 1 radian where θ = ωτ. At room temperature, $\tau \approx 10^{-13}$ sec to 10^{-15} sec, which puts a lower limit on ω and hence on B. The collision time, τ, can be increased (and thus ω decreased) if we go to lower temperatures and purer materials.

Homework problem 32 *considers cyclotron resonance.*