

Lecture 15. Introduction to k.p theory

Electrons in a solid are described by the single electron Schrödinger equation with a potential V :

$$H\psi = \left(\frac{p^2}{2m} + V \right) \psi = E\psi$$

If V is a periodic potential with symmetries that obey a crystal's given symmetry, the wavefunction ψ has to obey Bloch's theorem:

$$\psi_{n,k}(\vec{r}) = e^{i\vec{k}\vec{r}} u_{n,k}(\vec{r})$$

Here k is the electron wavenumber and n is the band index. $u_{n,k}(\vec{r})$ should also have the same periodicity as the crystal.

When H acts on this wavefunction, one obtains:

$$H\psi_{n,k}(\vec{r}) = \left(\frac{p^2}{2m} + V \right) e^{i\vec{k}\vec{r}} u_{n,k}(\vec{r})$$

For simplicity, and without loss of generality, let us work in 1D where $p = -i\hbar\partial_x$:

$$\begin{aligned} H\psi_{n,k}(x) &= \frac{1}{2m} p^2 e^{ikx} u_{n,k}(x) + V e^{ikx} u_{n,k}(x) = \frac{\hat{p}}{2m} (\hbar k e^{ikx} u_{n,k} + e^{ikx} \hat{p} u_{n,k}) + V e^{ikx} u_{n,k} \\ &= \frac{1}{2m} (\hbar(\hat{p} \cdot k) e^{ikx} u_{n,k} + \hbar^2 k^2 e^{ikx} u_{n,k} + e^{ikx} p^2 u_{n,k} + \hbar e^{ikx} (k \cdot \hat{p}) u_{n,k}) + V e^{ikx} u_{n,k} = E e^{ikx} u_{n,k} \end{aligned}$$

Note that k is a simple vector that characterizes the periodicity of the wavefunction, where \hat{p} is the momentum operator (i.e. $\hat{p} \neq \hbar k$).

We can now rewrite the expression for the Hamiltonian, by rearranging terms as:

$$\frac{p^2}{2m} u_{n,k} + \frac{\hbar}{m} (k \cdot \hat{p}) u_{n,k} + \frac{\hbar^2 k^2}{2m} u_{n,k} + V u_{n,k} = E_{n,k} u_{n,k}$$

We define two separate terms:

$$H_0 = \frac{p^2}{2m} + V$$

And

$$H_k = \frac{\hbar}{m} (k \cdot \hat{p}) + \frac{\hbar^2 k^2}{2m}$$

H_0 is the free electron part of the Hamiltonian, and H_k is the k -dependent crystal Hamiltonian. This second term will be treated perturbatively.

k.p perturbation theory: a toy model with 2 bands

A perturbation treatment is the simplest way to compute the band dispersion of a material using the k.p formalism. For a given semiconductor system with 2 bands (conduction and valence) an optical spectroscopy measurement can allow on to extract the value of the energy gap. With this knowledge acquired beforehand, k.p theory allows a computation of the band dispersion in the vicinity of the band edges. Assume we have a system constituted of 2 bands located at $\pm E_g/2$ (mid gap in the zero-energy point)

Physically speaking, this means that the eigenvalues of the k-independent Hamiltonian for these two bands are $\pm E_g/2$.

$$H_0 u_{n,0} = \frac{E_g}{2} u_{n,0}$$

Applying first order degenerate perturbation yields:

$$\begin{pmatrix} E_n + \langle u_{n,0} | H_k | u_{n,0} \rangle & \langle u_{n,0} | H_k | u_{m,0} \rangle \\ \langle u_{m,0} | H_k | u_{n,0} \rangle & E_m + \langle u_{m,0} | H_k | u_{m,0} \rangle \end{pmatrix}$$

Assuming the two bands have opposite parity, as is the case with most semiconductors. The operator \hat{p} acting on each Bloch function will yield its derivative, so that the \hat{p} dependent diagonal terms vanish by symmetry:

$$\langle u_{n,0} | H_k | u_{n,0} \rangle = \frac{\hbar^2 k^2}{2m} + \frac{\hbar}{m} k \langle u_{n,0} | \hat{p} | u_{n,0} \rangle = \frac{\hbar^2 k^2}{2m}$$

Also, the off-diagonal are particularly interesting to consider since they yield k-linear terms:

$$\langle u_{n,0} | H_k | u_{m,0} \rangle = \langle u_{m,0} | H_k | u_{n,0} \rangle = \frac{\hbar}{m} k \langle u_{n,0} | \hat{p} | u_{m,0} \rangle = \frac{\hbar}{m} k \cdot P$$

Here $P \equiv \langle u_{n,0} | H_k | u_{m,0} \rangle$ is simply a real number referred to as the k.p matrix element. We will later examine its true meaning in a more realistic context. In this situation, it simply takes into account the ('repulsive?') interaction between the two bands considered.

So in the end, we have to diagonalize the following Hamiltonian to find the band structure of the material in the vicinity of the band edge:

$$\begin{pmatrix} \frac{E_g}{2} + \frac{\hbar^2 k^2}{2m} & \frac{\hbar}{m} k \cdot P \\ \frac{\hbar}{m} k \cdot P & -\frac{E_g}{2} + \frac{\hbar^2 k^2}{2m} \end{pmatrix} \begin{pmatrix} u_{n,k} \\ u_{m,k} \end{pmatrix} = E_{n,k} \begin{pmatrix} u_{n,k} \\ u_{m,k} \end{pmatrix}$$

So we find,

$$E_{\pm,k} = \frac{\hbar^2 k^2}{2m} \pm \sqrt{\left(\frac{E_g}{2}\right)^2 + \left(\frac{\hbar}{m} k \cdot P\right)^2}$$

The energy has a parabolic term and a term that resembles a Dirac dispersion with velocity,

$$v = \frac{P}{m}$$

Typically, in semiconductors, the 2 bands result from cation/anion s and $p_{x,y}$ orbitals, so that,

$$\frac{\langle u_{n,0} | \hat{p} | u_{m,0} \rangle}{m} = \frac{\langle S | \hat{p} | f(X, Y) \rangle}{m}$$

The approximate order of magnitude of this matrix element is well known to be $v_c \sim 10^6 \text{m/s}$ or $\hbar v_c \approx 6.6 \text{eV}\text{\AA}$. Conversely, since m is the free-electron mass, the k^2 term coefficient is about $3.7 \text{eV}\text{\AA}^2$.

In Fig. 1 we plot $E_{\pm,k}$ for different values of $E_g/2$. The Dirac-like shape of the band structure is indeed remarkable.

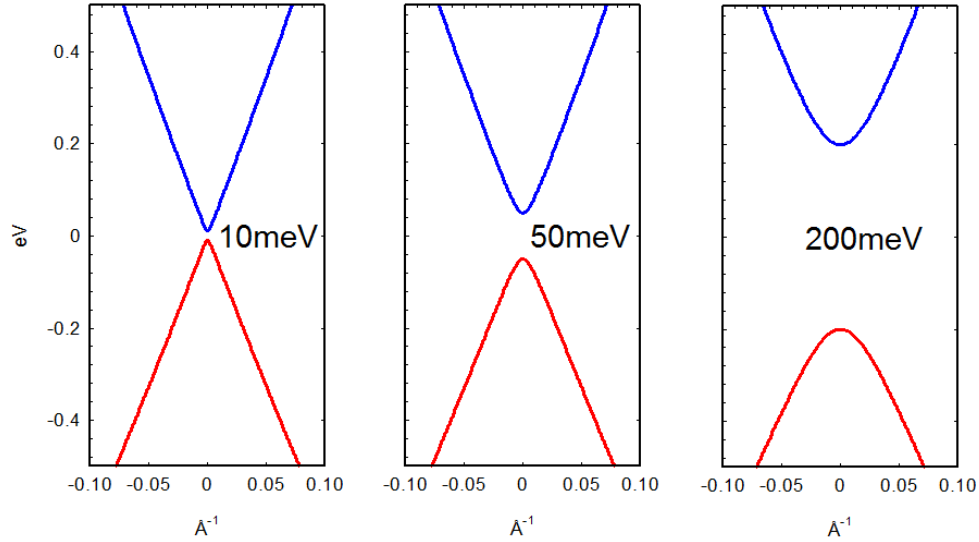


FIG 1. Dispersion obtained from the 2-band k.p method for different values of the half-energy gap.

A minor difference between Dirac fermions resulting from k.p treatments and ideal Dirac cones is the presence of both linearly dispersing components and parabolic components. You will examine the implications of the parabolic components on the dispersion in the homework assignment.

Linear dispersions in condensed-matter

Linear Dirac-like dispersions have been known to occur in semiconductors as early as the mid-1950s. One of the first treatments of the band structure of a semiconductor (InSb) came in a paper by Evan O. Kane (G.E. Research Lab, N.Y.) who used a k.p formalism applied to the bands of III-V materials. Kane noticed that while the band structure of InSb is parabolic at low energies and quite similar to that of Ge for example, it asymptotically became linear far away from the band edge.

From a practical point-of-view, most semiconductors usually host a non-negligible amount of defects such as atomic vacancies and anti-site defects. The most immediate impact of such defects is the fact they result in free carriers. As long as the amount of defects is small enough to not cause a renormalization of the band structure, but large enough to yield free carriers, one can represent their impact by a finite carrier filling (or emptying) of the energy levels of the system. Typically, one finds between 10^{14} and 10^{19}cm^{-3} carriers per cm^{-3} in most semiconductors. A record low carrier concentration for Ge for example was 10^9cm^{-3} but is exceptionally difficult to reach. A record low for HgTe is 10^{12}cm^{-3} but is also extremely challenging to reach. In general, these records require the use of industrial grade synthesis equipment and operation with highly optimized growth parameters and cleanliness.

Thus overall the range of carrier densities that typically occur in materials gives a range of Fermi energies that are possible and interesting namely, $\sim 0\text{meV}$ and $\sim 100\text{meV}$ above the mid-gap. Most optical and electronic applications almost require the Fermi level to be in this range. If we fix E_f to 300meV in Fig. 1 again, one can easily notice that for larger gap systems, the band edge becomes more and more parabolic. *Thus, a general consequence of $k.p$ theory with the assumptions used above is that narrow gap semiconductors always have a Dirac-like 'non-parabolic' dispersion.*

Consequences on transport and optical properties

The most immediate consequence on transport and optical properties is the fact that the effective mass becomes energy dependent. As we saw in HW1, one can write the effective mass as:

$$m^* = \hbar^2 \left(\frac{d^2 E_f}{dk^2} \right)^{-1}$$

Here $A_f = \pi k_f^2$ is the area of the Fermi surface

With, the Fermi energy for the conduction band given by:

$$E_f = \frac{\hbar^2 k^2}{2m} + \sqrt{\left(\frac{E_g}{2}\right)^2 + (\hbar v k)^2}$$

We get,

$$m^* = \hbar^2 \left(\frac{\hbar^2}{m} + \frac{(\hbar v)^2}{\left[\left(\frac{E_g}{2}\right)^2 + (\hbar v k)^2\right]^{1/2}} - \frac{(\hbar v)^4 k^2}{\left[\left(\frac{E_g}{2}\right)^2 + (\hbar v k)^2\right]^{3/2}} \right)^{-1}$$

$$m^* = \left(\frac{1}{m} + \frac{(v)^2 \left[\left(\frac{E_g}{2}\right)^2 + (\hbar v k)^2\right]}{\left[\left(\frac{E_g}{2}\right)^2 + (\hbar v k)^2\right]^{3/2}} - \frac{v^4 (\hbar k)^2}{\left[\left(\frac{E_g}{2}\right)^2 + (\hbar v k)^2\right]^{3/2}} \right)^{-1}$$

Finally,

$$m^* = \left(\frac{1}{m} + \frac{\left(\frac{E_g v}{2}\right)^2}{\left[\left(\frac{E_g}{2}\right)^2 + (\hbar v k)^2\right]^{3/2}} \right)^{-1}$$

Notice that at $k=0$,

$$m^* = \left(\frac{1}{m} + \frac{2v^2}{E_g} \right)^{-1}$$

For $E_g/2=10meV$ and $v=10^6m/s$, we get,

$$m^* = \left(\frac{1}{m} + \frac{2v^2}{E_g} \right)^{-1} = \left(\frac{1}{m} + \frac{1}{0.0018m} \right)^{-1} = 0.0018m$$

It is interesting to note that for typical narrow-gap (and even ‘mid-gap’) systems, the free electron term is negligible, and we can comfortably use the following formula for the two band k.p effective mass:

$$m^* = \frac{E_g}{2v^2}$$

Recalling the resemblance between this formula rewritten as:

$$\frac{E_g}{2v^2} = m^*v^2$$

and, Einstein’s energy-mass relation, one can easily get an idea about the exciting parallels that can be made between condensed-matter and high-energy physics.