Effective mass, holes, energy band diagram

LECTURE 3

- Material classification
- Effective mass
- Parabolic Band Approximation
- Holes
- Bands in real semiconductors
- Constant-energy surfaces
- Energy band diagram

Sec. 2.7

Semiconductor, metal, or insulator?

Our N=10 example is for one-electron primitive cells and gives N states per BAND.

Allowing for spin there are 2N states per band

Silicon has 2 atoms per primitive cell, with 4 valence electrons in each atom,

i.e., 8 electrons per primitive cell and 8N valence electrons in total.

Therefore, the first 4 bands are completely filled (at 0K).

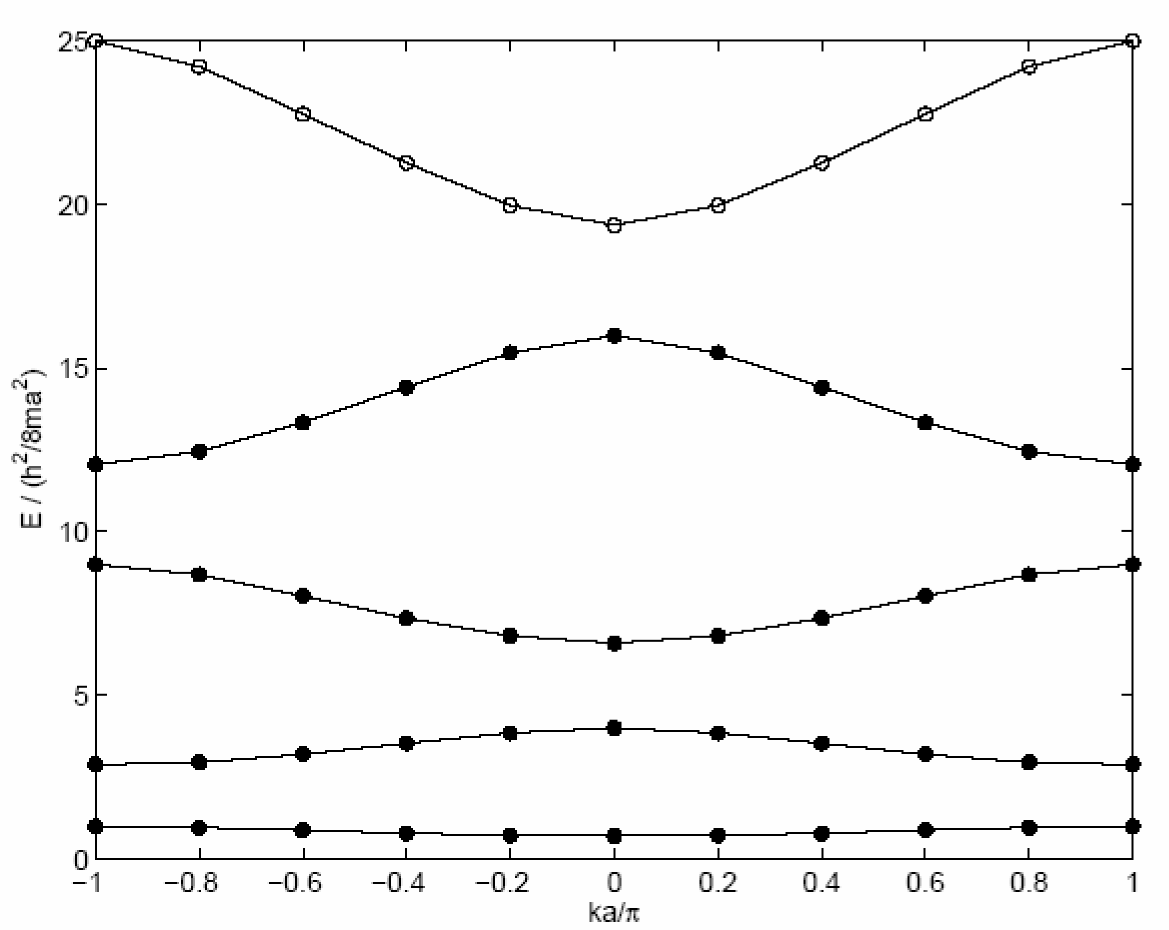
What happens at T > 0K ?

Where is the BANDGAP?

One possibility for a metal is that the material has 3N valence electrons.

Why does this make a metal?

What makes an insulator?



Sec. 2.9

Crystal momentum and external force

$$\frac{dE}{dt} = F_{x,\,\mathrm{ext}}\frac{dx}{dt} = F_{x,\,\mathrm{ext}}\,v_x$$

Energy gain from an external force

e.g., F=

$$v_x = \frac{1}{\hbar}\frac{dE}{dk_x}\,.$$

group velocity ≡

Implications of using this velocity?

$$\frac{dE}{dt} = \frac{dE}{dk_x}\frac{dk_x}{dt}\,,$$

Chain Rule

ħk is the

$$F_{x,\,\mathrm{ext}} = \frac{d(\hbar k_x)}{dt}\,.$$

The crystal momentum changes due to

Sec. 2.9

Effective mass

$$a_x = \frac{dv_x}{dt} = \frac{1}{\hbar}\frac{d^2E}{dk_x^2}\frac{dk_x}{dt} = \frac{1}{\hbar^2}\frac{d^2E}{dk_x^2}\frac{d(\hbar k_x)}{dt}$$

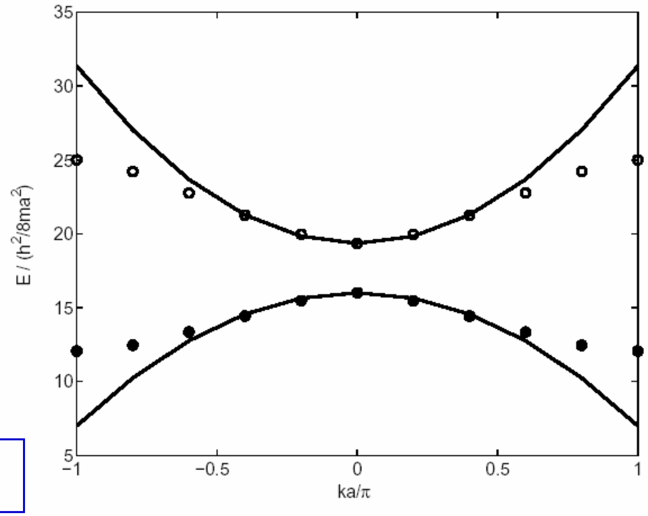
$$a_x = \left[\frac{1}{\hbar^2}\frac{d^2E}{dk_x^2}\right] F_{x,\,\mathrm{ext}} \quad \Longrightarrow \quad m_x^*(E) = \left[\frac{1}{\hbar^2}\frac{d^2E}{dk_x^2}\right]^{-1}$$

What is the sign of m* at the top of the VB?

What does this mean?

If m* is constant, we have a band.

Apply such an approximation to our toy bands.

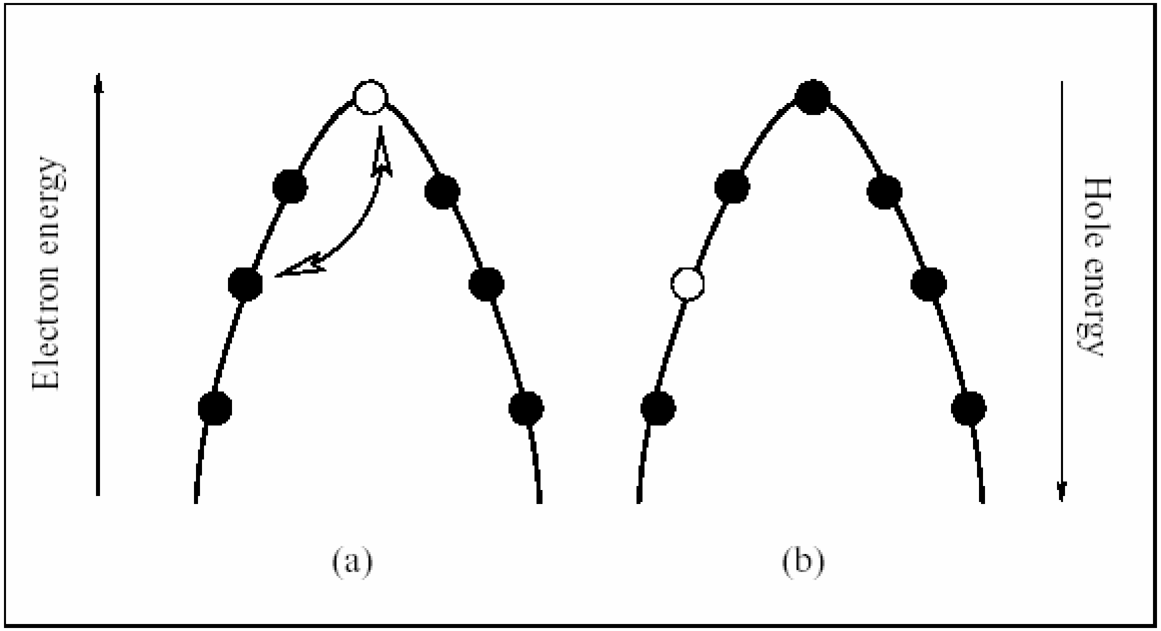


Is it useful to have an approximation that only works near the band extrema?

What is a useful equation for the conduction band?

Sec. 2.9.1

Holes



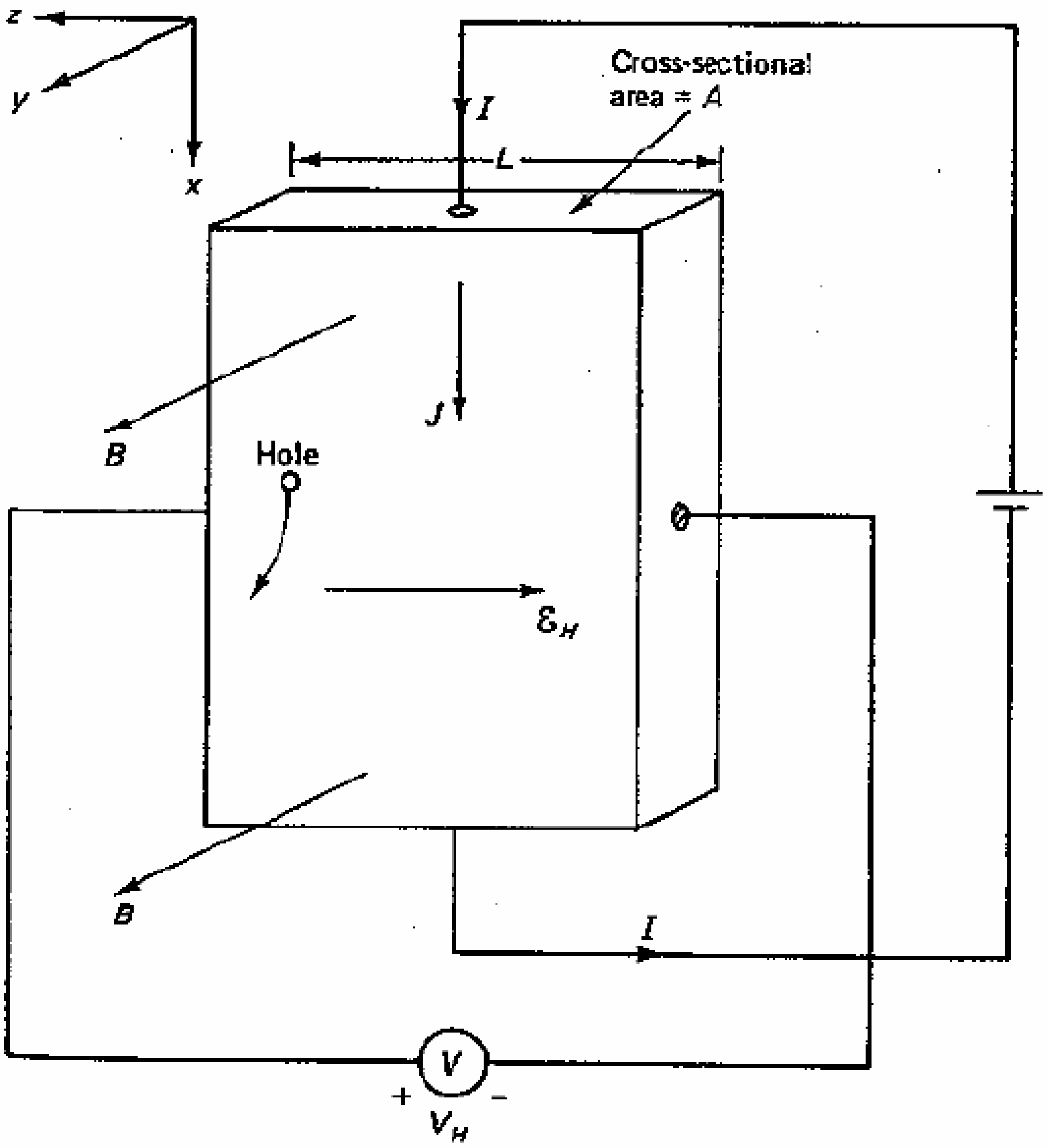
What is the x-axis on this plot?

We can view this excitation event as EITHER a VB electron gaining energy OR as a gaining energy.

What is the advantage of choosing the latter viewpoint?

What is the charge on a hole?

The Hall Effect



F =

What is the Hall-Effect voltage when:

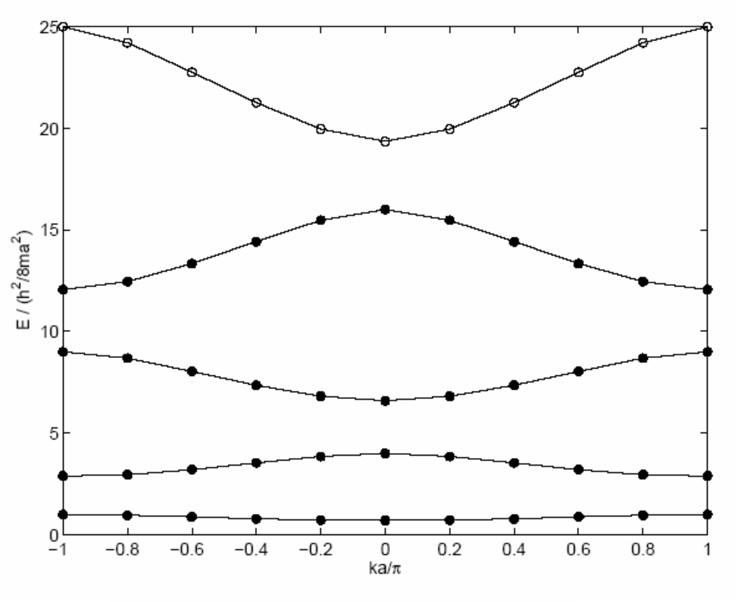
1. n=p
2. n>p
3. n<p ?

n and p are, respectively, the concentrations of

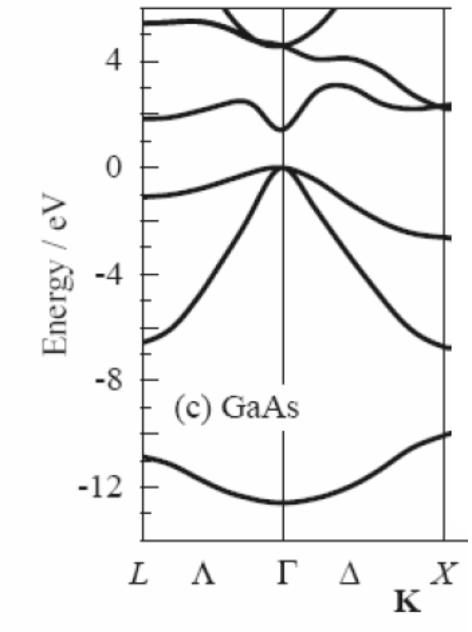
What are their units in 3-D?

Sec. 2.8

Energy bands in real materials



This is what we have from our toy model.



This is what you get for real gallium arsenide.

Note:

- 4 (FOUR) bands for valence electrons
- Strange notation for Bloch wavevector

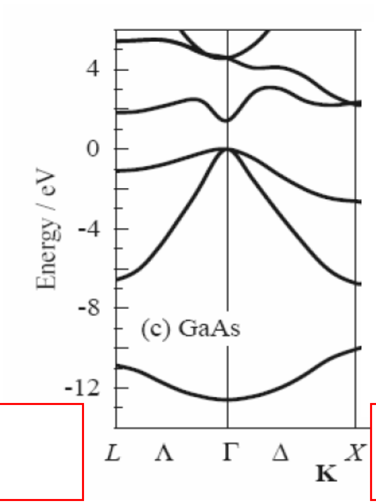
Identify the valence bands.

Why are the curves asymmetrical about the Γ point?

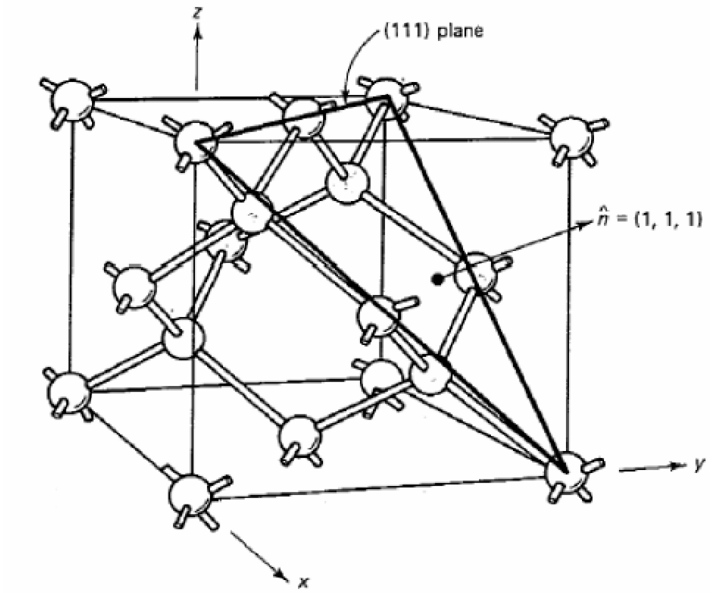
Sec. 2.8

Labeling directions and planes

Label directions using
Miller indices.



The directions in k-space (reciprocal space) are perpendicular to the corresponding planes in real space.



What is the label for the front face?

Sec.
2.10

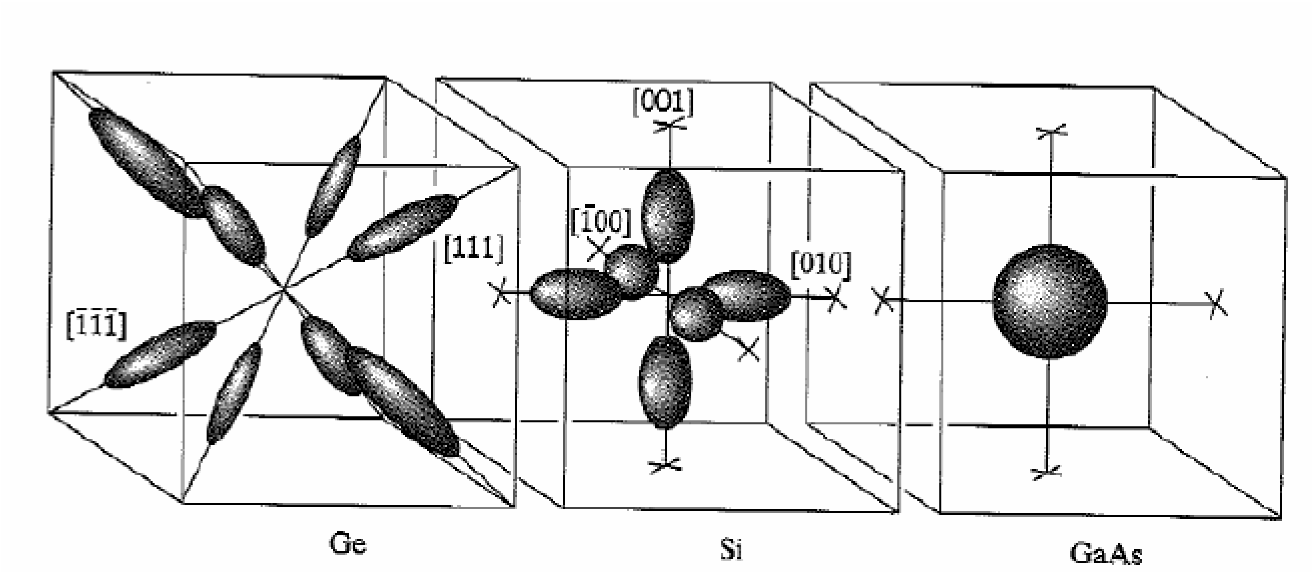
Constant-energy surfaces

In 3-D structures, the parabolic-effective-mass concept leads naturally to

$$E - E_{C0} = \frac{\hbar^2}{2}\boxed{\qquad\qquad\qquad} ,$$

Can you see how degeneracies can occur?

Constant-energy surfaces for electrons in the CB



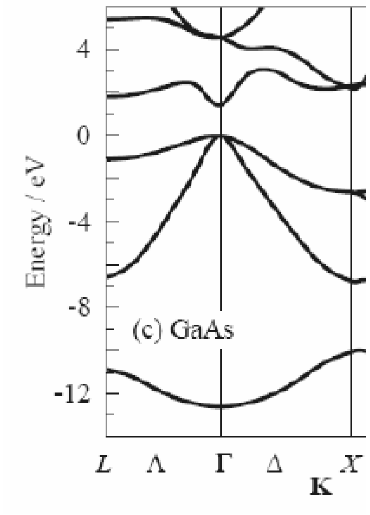
Which axis corresponds to k_x?

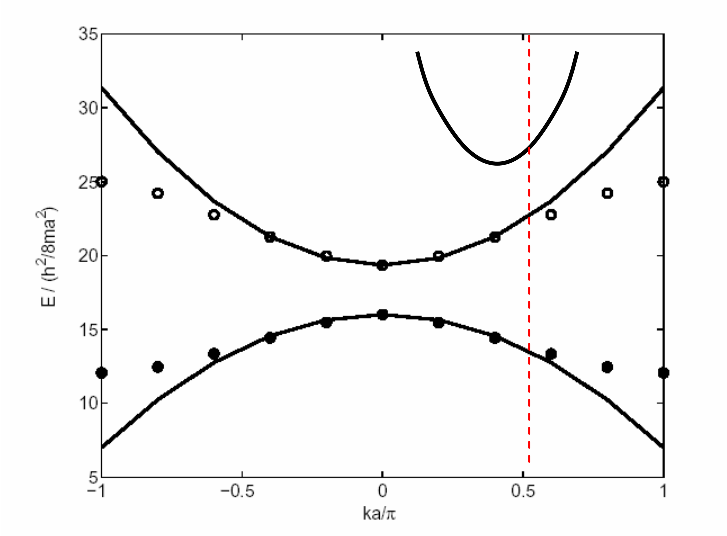
How many values of m_e^* for (a) Si, (b) GaAs ?

Sec. 2.12

Potential energy

Microscopically:

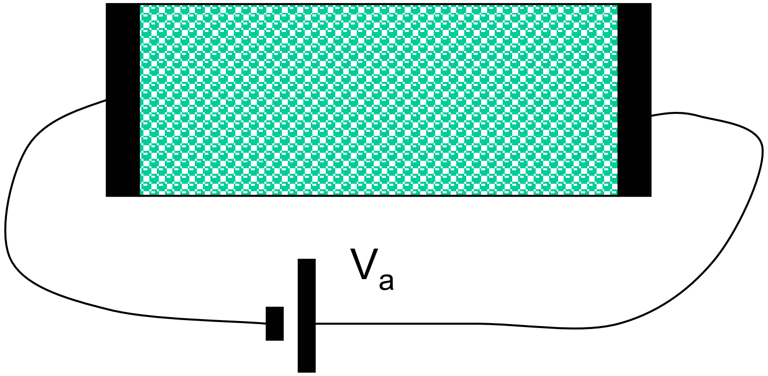




$$E_\nu(k) = E_{C0} + \frac{\hbar^2 k^2}{2m^*}$$

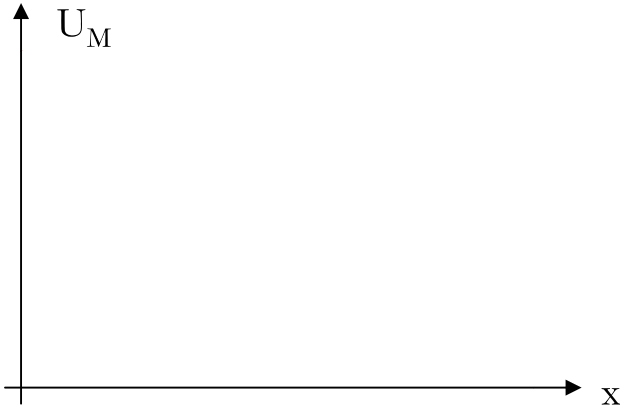
- What is v ?
- Where is E_{C0} for v = 1 ?
- Physically, what is E_{C0} ?

Macroscopically:



What is $U_M(x)$?

Sketch it for this case.



Sec. 2.12

Energy band diagram

Add in the macroscopic potential energy

$$
\begin{aligned}
E &= U_M(x) + E_{C0} + \frac{\hbar^2 k^2}{2m^*} \\
&\equiv E_C(x) + \frac{\hbar^2 k^2}{2m^*} \,,
\end{aligned}
$$