

# Homework 6 Solutions

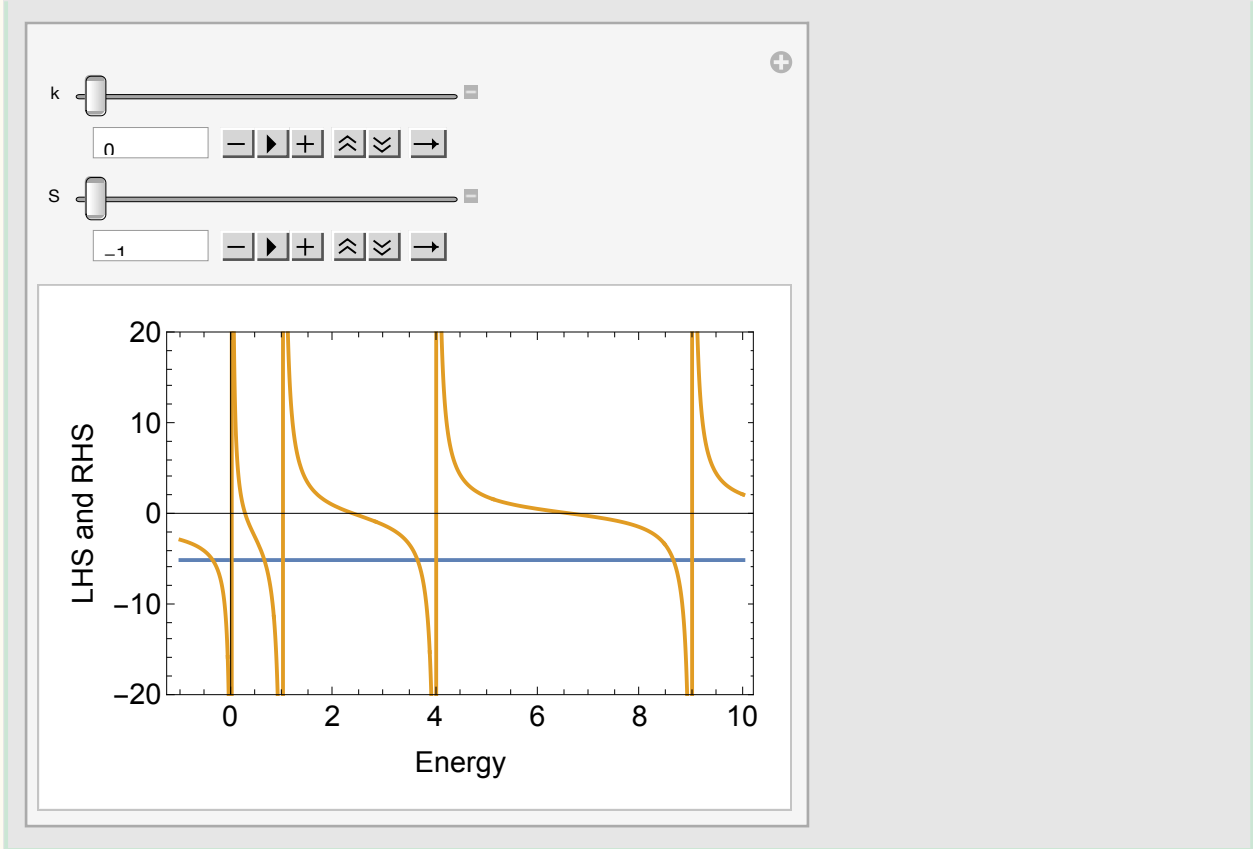
## ECE 4070/MSE 5470: Physics of Semiconductors and Nanostructures Debdeep Jena

### ■ 6.1) The Kronig-Penney Model

In[1]:=

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(* The Kronig-Penney model can be written in a non-dimensional form as  $\frac{2*\pi^2*\hbar^2}{m*S*a} =$   
 $\sum_{n=-N/2}^{N/2} \frac{1}{en - (k+n)^2}$  where S is the Delta function strength,  
a is the lattice constant, en is the dimensionless energy in units  
of  $4*\frac{\hbar^2}{2*m}*\left(\frac{\pi}{a}\right)^2$ , and k is the dimensionless wavevector in  $\frac{2\pi}{a}$  units*)  
rhs[en_, k_, N_] :=  $\sum_{n=-N/2}^{N/2} \frac{1}{en - (k + n)^2}$   
(* Positive or repulsive Delta comb, dimensionless,  
n in integers, k in  $\frac{2\pi}{a}$  units, and en in  $4*\frac{\hbar^2}{2*m}*\left(\frac{\pi}{a}\right)^2$  units,  
also the Trace of the Green's Function *)  
lhs[a_, S_] :=  $\frac{2 * \pi^2 * \left(\frac{6.63*10^{-34}}{2*\pi}\right)^2}{(9.1 * 10^{-31} * S * 1.6 * 10^{-19} * 10^{-9} * a * 10^{-9})}$   
(* Also dimensionless,  $\frac{2*\pi^2*\hbar^2}{m*S*a}$ , S in eV.nm and a in nm *)  
Manipulate[Plot[{lhs[0.3, S], rhs[en, k, 10]}, {en, -1, 10},  
PlotRange -> {-20, 20}, Frame -> True, FrameLabel -> {"Energy", "LHS and RHS"},  
PlotStyle -> Thick, BaseStyle -> {FontSize -> 15}], {k, 0, 1}, {S, -1, -10}]  
(* Pictorial solution of the Kronig-Penney Model *)
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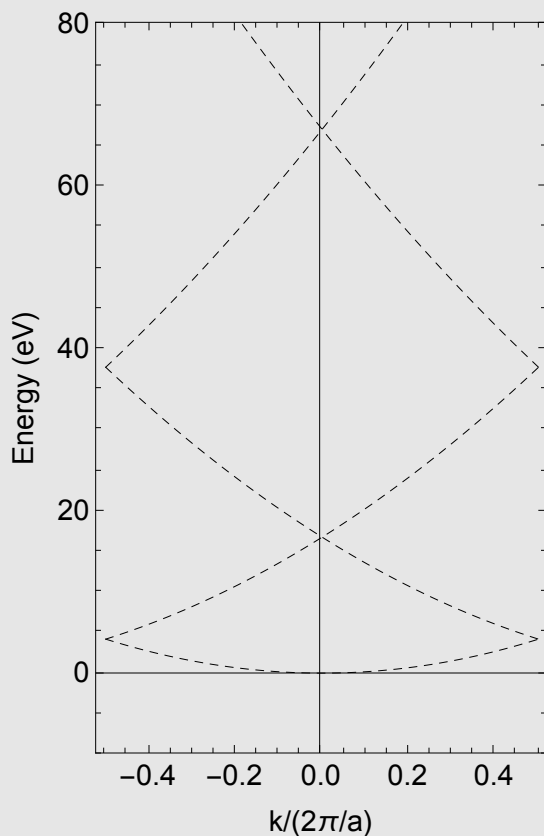
Out[3]=



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In[4]:=
F[a_] := 4 *  $\frac{\left(\frac{6.63 \cdot 10^{-34}}{2 \cdot \pi}\right)^2}{2 \cdot 9.1 \cdot 10^{-31} \cdot 1.6 \cdot 10^{-19}} \cdot \left(\frac{\pi}{a \cdot 10^{-9}}\right)^2$ ;
(* Natural energy scale,  $4 \cdot \frac{\hbar^2}{2 \cdot m} \cdot \left(\frac{\pi}{a}\right)^2$ , expressed in eV *)
e0k[n_, k_, a_] := (k + n)^2 * F[a];
(* Nearly free electron energy "bands" in eV *)
Plot[{e0k[0, k, 0.3], e0k[1, k, 0.3], e0k[-1, k, 0.3],
      e0k[+2, k, 0.3], e0k[-2, k, 0.3]}, {k, -0.5, 0.5}, PlotRange -> {-10, 80},
      Frame -> True, FrameLabel -> {"k/(2π/a)", "Energy (eV)"},
      PlotStyle -> {{Black, Dashed, Thin}, {Black, Dashed, Thin},
                   {Black, Dashed, Thin}, {Black, Dashed, Thin}, {Black, Dashed, Thin}},
      BaseStyle -> {FontSize -> 15}, AspectRatio -> GoldenRatio]
(* Nearly Free electron Bandstructure: the Lattice constant is 0.3 nm *)

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## Nearly free electron Bandstructure

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In[7]:=
ek[a_, S_, N_, k_] := NSolve[lhs[a, S] == rhs[en, k, N], en];
(* Solve for E(k) - The Kronig Penney Solution in dimensionless form *)
bands[num_, a_, S_, N_, k_] := F[a] * Part[Sort[ek[a, S, N, k]], num][[1]][[2]];
(* Sort the bands and put back the dimensions
   by multiplying the characteristic energy scale *)

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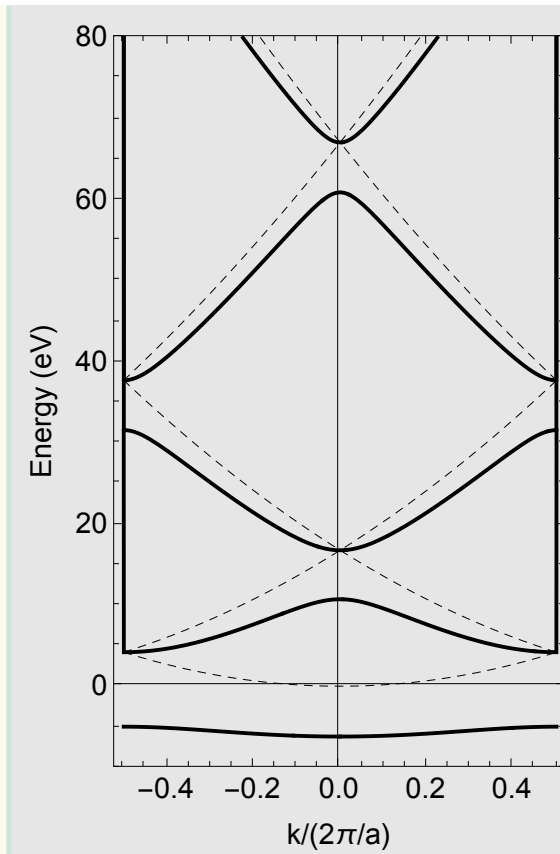
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(* bands[num_,a_,S_,N_,k_] *)
(* "large" delta function strength of S=-1 eV.nm,
lattice constant of a=0.3 nm *)
KP1 = Plot[{e0k[0, k, 0.3], e0k[1, k, 0.3], e0k[-1, k, 0.3], e0k[+2, k, 0.3],
  e0k[-2, k, 0.3], bands[1, 0.3, -1, 10, k], bands[2, 0.3, -1, 10, k],
  bands[3, 0.3, -1, 10, k], bands[4, 0.3, -1, 10, k], bands[5, 0.3, -1, 10, k]},
{k, -0.5, 0.5}, PlotRange → {-10, 80}, Frame → True,
FrameLabel → {"k/(2π/a)", "Energy (eV)"},
PlotStyle → {{Black, Dashed, Thin}, {Black, Dashed, Thin}, {Black, Dashed, Thin},
{Black, Dashed, Thin}, {Black, Dashed, Thin}, {Black, Thick},
{Black, Thick}, {Black, Thick}, {Black, Thick}},
BaseStyle → {FontSize → 15}, AspectRatio → GoldenRatio]
(* "smaller" delta function strength of S=-0.2 eV.nm,
lattice constant of a=0.3 nm *)
KP2 = Plot[{e0k[0, k, 0.3], e0k[1, k, 0.3], e0k[-1, k, 0.3],
  e0k[+2, k, 0.3], e0k[-2, k, 0.3], bands[1, 0.3, -0.2, 10, k],
  bands[2, 0.3, -0.2, 10, k], bands[3, 0.3, -0.2, 10, k],
  bands[4, 0.3, -0.2, 10, k], bands[5, 0.3, -0.2, 10, k]}, {k, -0.5, 0.5},
PlotRange → {-10, 80}, Frame → True, FrameLabel → {"k/(2π/a)", "Energy (eV)"},
PlotStyle → {{Black, Dashed, Thin}, {Black, Dashed, Thin}, {Black, Dashed, Thin},
{Black, Dashed, Thin}, {Black, Dashed, Thin}, {Black, Thick},
{Black, Thick}, {Black, Thick}, {Black, Thick}},
BaseStyle → {FontSize → 15}, AspectRatio → GoldenRatio]
(* "large" delta function strength of S=-1 eV.nm,
"large" lattice constant of a=0.5 nm *)
KP3 = Plot[{e0k[0, k, 0.5], e0k[1, k, 0.5], e0k[-1, k, 0.5], e0k[+2, k, 0.5],
  e0k[-2, k, 0.5], e0k[+3, k, 0.5], e0k[-3, k, 0.5], e0k[+4, k, 0.5],
  e0k[-4, k, 0.5], bands[1, 0.5, -1, 10, k], bands[2, 0.5, -1, 10, k],
  bands[3, 0.5, -1, 10, k], bands[4, 0.5, -1, 10, k], bands[5, 0.5, -1, 10, k],
  bands[6, 0.5, -1, 10, k], bands[7, 0.5, -1, 10, k], bands[8, 0.5, -1, 10, k]},
{k, -0.5, 0.5}, PlotRange → {-10, 80}, Frame → True,
FrameLabel → {"k/(2π/a)", "Energy (eV)"},
PlotStyle → {{Black, Dashed, Thin}, {Black, Dashed, Thin}, {Black, Dashed, Thin},
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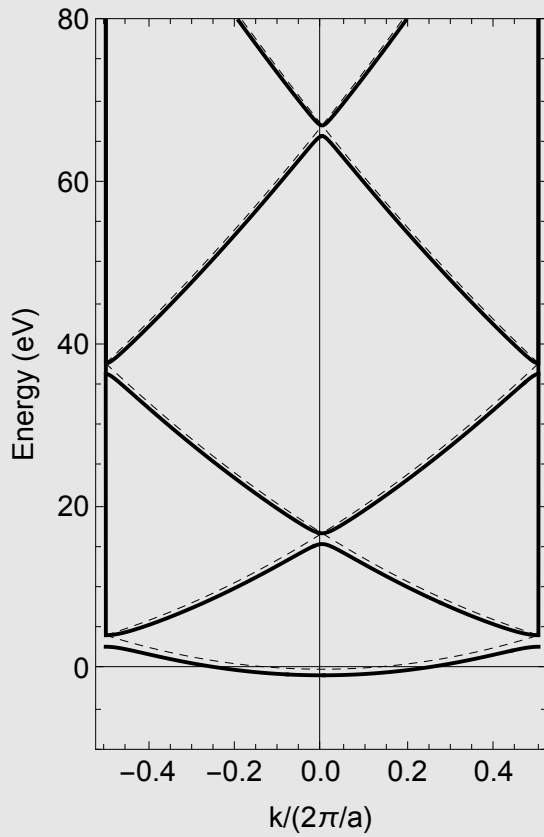
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S=-1 eV.nm

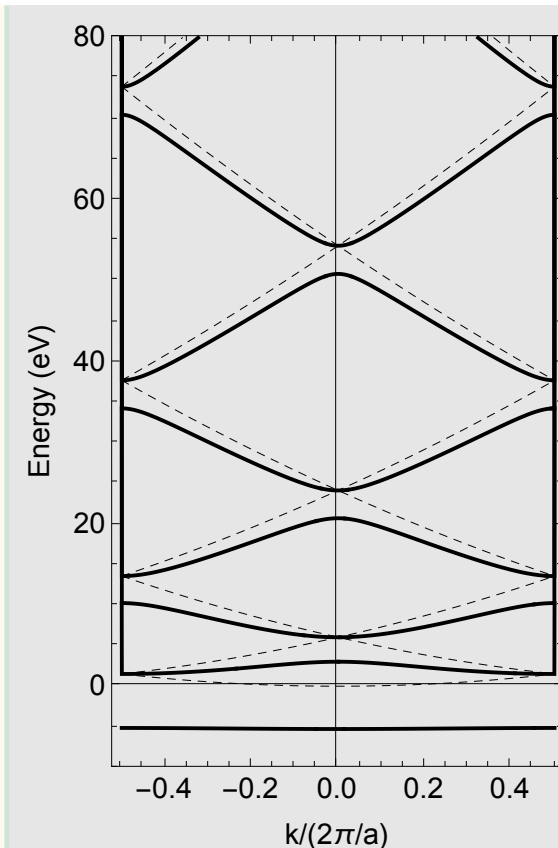
S=-0.2 eV.nm



$S = -1$  eV.nm  
(Solution to 6.1a)



$S = -0.2 \text{ eV.nm}$   
(Extra for illustration)



Solutions 6.1 b, c:

For Semiconductor A,  $4N$  states are occupied, each band has  $2N$  states  $\Rightarrow$  2 lowest bands occupied  $\Rightarrow$  Gap is between 2nd and 3rd bands.  $\Rightarrow$  Lowest “fundamental” gap is at  $k=0$ , or the Gamma point.

For Semiconductor B,  $6N$  electrons  $\Rightarrow$  3 lowest bands are occupied.  $\Rightarrow$  Lowest “fundamental” gap is at the 1st BZ edge.

```
(* Bandgaps for all k's and bands *)
Gaps[n_, a_, S_, N_, k_] := bands[n+1, a, S, N, k] - bands[n, a, S, N, k];
(* Bandgaps at the Gamma-Point at k=0 *)
Print["The first gap is at  $k=\pm\frac{\pi}{a}$ , and is  $E_{n=2}(k=\frac{\pi}{a}) - E_{n=1}(k=\frac{\pi}{a}) =$ ",
      Gaps[1, 0.3, -1, 10, 0.499], " eV"];
Print["The second gap is at  $k=0$ , and is  $E_{n=3}(k=0) - E_{n=2}(k=0) =$ ",
      Gaps[2, 0.3, -1, 10, 0.01], " eV"];
Print["The third gap is at  $k=\pm\frac{\pi}{a}$ , and is  $E_{n=4}(k=\frac{\pi}{a}) - E_{n=3}(k=\frac{\pi}{a}) =$ ",
      Gaps[3, 0.3, -1, 10, 0.499], " eV"];
Print["The fourth gap is at  $k=0$ , and is  $E_{n=5}(k=0) - E_{n=4}(k=0) =$ ",
      Gaps[4, 0.3, -1, 10, 0.01], " eV"];
```

The first gap is at  $k=\pm\frac{\pi}{a}$ , and is  $E_{n=2}(k=\frac{\pi}{a}) - E_{n=1}(k=\frac{\pi}{a}) = 9.18598$  eV

The second gap is at  $k=0$ , and is  $E_{n=3}(k=0) - E_{n=2}(k=0) = 6.0779$  eV **A: Gap energy**

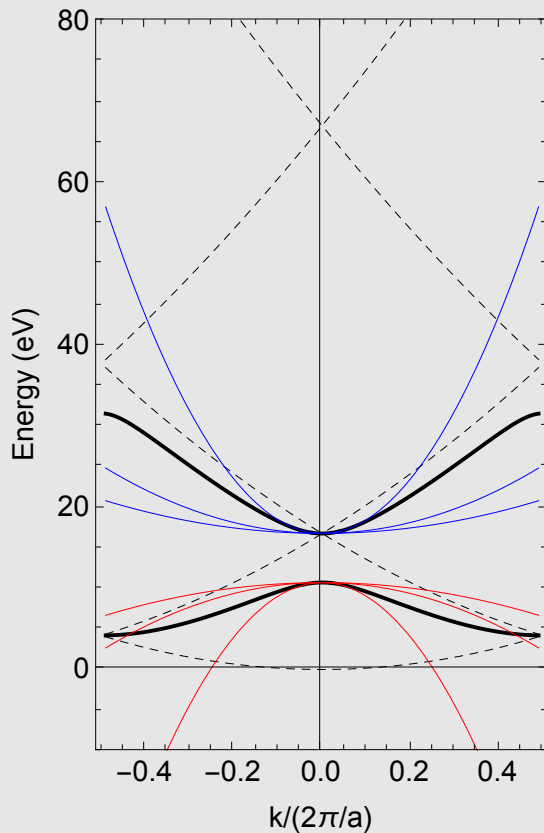
The third gap is at  $k=\pm\frac{\pi}{a}$ , and is  $E_{n=4}(k=\frac{\pi}{a}) - E_{n=3}(k=\frac{\pi}{a}) = 6.14368$  eV **B: Gap energy**

The fourth gap is at  $k=0$ , and is  $E_{n=5}(k=0) - E_{n=4}(k=0) = 6.30772$  eV

```

Plot[{{e0k[0, k, 0.3], e0k[1, k, 0.3], e0k[-1, k, 0.3], e0k[+2, k, 0.3],
      e0k[-2, k, 0.3], bands[2, 0.3, -1, 10, k], bands[2, 0.3, -1, 10, 0.01] -  $\frac{F[0.3]}{1.0} * k^2$ ,
      bands[2, 0.3, -1, 10, 0.01] -  $\frac{F[0.3]}{0.5} * k^2$ , bands[2, 0.3, -1, 10, 0.01] -  $\frac{F[0.3]}{0.1} * k^2$ ,
      bands[3, 0.3, -1, 10, k], bands[3, 0.3, -1, 10, 0.01] +  $\frac{F[0.3]}{1.0} * k^2$ ,
      bands[3, 0.3, -1, 10, 0.01] +  $\frac{F[0.3]}{0.5} * k^2$ , bands[3, 0.3, -1, 10, 0.01] +  $\frac{F[0.3]}{0.1} * k^2$ },
  {k, -0.49, 0.49}, PlotRange -> {-10, 80}, Frame -> True,
  FrameLabel -> {"k/(2π/a)", "Energy (eV)"},
  PlotStyle -> {{Black, Dashed, Thin}, {Black, Dashed, Thin}, {Black, Dashed, Thin}, {Black, Dashed, Thin},
  {Black, Dashed, Thin}, {Black, Dashed, Thin}, {Black, Thick}, {Red, Thin}, {Red, Thin},
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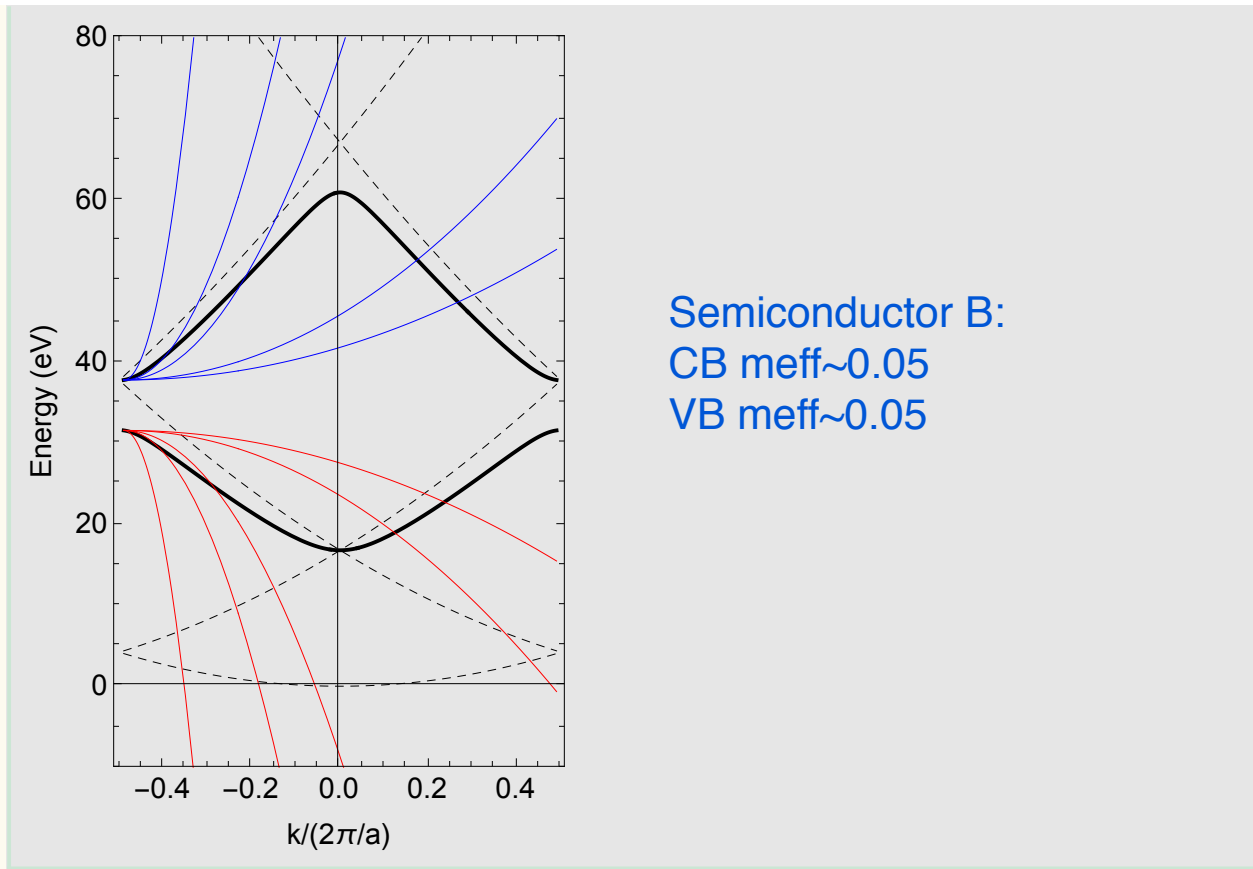
Semiconductor A:  
 CB  $m_{\text{eff}} \sim 0.1$   
 VB  $m_{\text{eff}} \sim 0.1$



```

Plot[ {e0k[0, k, 0.3], e0k[1, k, 0.3], e0k[-1, k, 0.3],
      e0k[+2, k, 0.3], e0k[-2, k, 0.3], bands[3, 0.3, -1, 10, k],
      bands[3, 0.3, -1, 10, 0.49] -  $\frac{F[0.3]}{1.0} * (k + 0.49)^2$ ,
      bands[3, 0.3, -1, 10, 0.49] -  $\frac{F[0.3]}{0.5} * (k + 0.49)^2$ ,
      bands[3, 0.3, -1, 10, 0.49] -  $\frac{F[0.3]}{0.1} * (k + 0.49)^2$ ,
      bands[3, 0.3, -1, 10, 0.49] -  $\frac{F[0.3]}{0.05} * (k + 0.49)^2$ ,
      bands[3, 0.3, -1, 10, 0.49] -  $\frac{F[0.3]}{0.01} * (k + 0.49)^2$ ,
      bands[4, 0.3, -1, 10, k], bands[4, 0.3, -1, 10, 0.49] +  $\frac{F[0.3]}{1.0} * (k + 0.49)^2$ ,
      bands[4, 0.3, -1, 10, 0.49] +  $\frac{F[0.3]}{0.5} * (k + 0.49)^2$ ,
      bands[4, 0.3, -1, 10, 0.49] +  $\frac{F[0.3]}{0.1} * (k + 0.49)^2$ ,
      bands[4, 0.3, -1, 10, 0.49] +  $\frac{F[0.3]}{0.05} * (k + 0.49)^2$ ,
      bands[4, 0.3, -1, 10, 0.49] +  $\frac{F[0.3]}{0.01} * (k + 0.49)^2$ },
      {k, -0.49, 0.49}, PlotRange -> {-10, 80}, Frame -> True,
      FrameLabel -> {"k/(2π/a)", "Energy (eV)"},
      PlotStyle -> {{Black, Dashed, Thin}, {Black, Dashed, Thin}, {Black, Dashed, Thin},
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                    {Red, Thin}, {Red, Thin}, {Red, Thin}, {Red, Thin}, {Black, Thick},
                    {Blue, Thin}, {Blue, Thin}, {Blue, Thin}, {Blue, Thin}, {Blue, Thin}},
      BaseStyle -> {FontSize -> 15}, AspectRatio -> GoldenRatio]

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**The trend of bandgaps and effective masses:  
With increase of the atomic number the band edge effective masses should decrease.**

## Problem 6.2

An easy way to do this problem is to rotate the coordinate system such that the inverse effective mass matrix is diagonal in the new coordinate system. Let the appropriate rotation matrix and the resulting diagonal matrix be:

$$R.M^{-1}.R^{-1} = \begin{bmatrix} 1/m_{xx} & 0 & 0 \\ 0 & 1/m_{yy} & 0 \\ 0 & 0 & 1/m_{zz} \end{bmatrix}$$

This implies that (just like in the case of Silicon) that the density of states effective mass is,

$$\begin{aligned} m_e &= (m_{xx}m_{yy}m_{zz})^{1/3} = \frac{1}{\det(R.M^{-1}.R^{-1})^{1/3}} = \left[ \frac{1}{\det(R).\det(M^{-1}).\det(R^{-1})} \right]^{1/3} \\ &= \left[ \frac{\det(R)}{\det(R).\det(M^{-1})} \right]^{1/3} = \left[ \frac{1}{\det(M^{-1})} \right]^{1/3} = [\det(M)]^{1/3} \end{aligned}$$

## Problem 6.3

a) The answer follows from elementary vector calculus result that that the gradient of any function is perpendicular to the surface of constant value of the function. In the present case, the velocity is related to the gradient of the energy function,

$$\vec{v}_c(\vec{k}) = \frac{1}{\hbar} \nabla_{\vec{k}} E(\vec{k})$$

And therefore the velocity must be perpendicular to the surfaces of constant energy.

## Problem 6.4

a) First note that:  $|\vec{k}_{||}| = \frac{\vec{B} \cdot \vec{k}}{|\vec{B}|}$

Now take the dot product on both sides of the crystal momentum equation with the magnetic field to get:

$$\vec{B} \cdot \frac{d \hbar \vec{k}}{dt} = -e \vec{B} \cdot [ \vec{v}_c(\vec{k}) \times \vec{B} ]$$

$$\Rightarrow \vec{B} \cdot \frac{d \hbar \vec{k}}{dt} = 0$$

$$\Rightarrow \frac{d \vec{B} \cdot \vec{k}}{dt} = 0$$

$$\Rightarrow \frac{d |\vec{k}_{||}|}{dt} = 0$$

$$b) \frac{dE_c(\vec{k}(t))}{dt} = \frac{1}{\hbar} \nabla_{\vec{k}} E_c(\vec{k}(t)) \cdot \frac{d\hbar \vec{k}(t)}{dt} = \vec{v}_c(\vec{k}(t)) \cdot \left[ -e \left[ \vec{v}_c(\vec{k}(t)) \times \vec{B} \right] \right] = 0$$

c) The complete argument follows in two steps:

- i) Since the energy of the electron remains unchanged and equal to its initial value  $E_0$ , the motion in k-space of the electron must be confined to a constant energy surface corresponding to the initial energy  $E_0$  of the electron.
- ii) Since the component of its crystal momentum parallel to the magnetic field also remains unchanged and equal to its initial value  $\vec{k}_{||}$ , the motion in k-space of the electron must also be confined to the plane in k-space on which the components of all crystal momenta in the direction of the magnetic field is  $\vec{k}_{||}$  (convince yourself that this later condition defines a plane in k-space that is perpendicular to the magnetic field).

Since both (i) and (ii) above must be true, the desired result follows.

d) One can always write the vector  $\vec{r}(t)$  in terms of its components in two orthogonal directions: parallel and perpendicular to the magnetic field:

$$\vec{r}(t) = \vec{r}_{\perp}(t) + \vec{r}_{||}(t)$$

But:

$$\vec{r}_{||}(t) = \left[ \frac{\vec{r}(t) \cdot \vec{B}}{|\vec{B}|^2} \right] \vec{B}$$

Therefore:

$$\vec{r}_{\perp}(t) = \vec{r}(t) - \left[ \frac{\vec{r}(t) \cdot \vec{B}}{|\vec{B}|^2} \right] \vec{B}$$

e) Start from,

$$\frac{d\hbar \vec{k}}{dt} = -e \left[ \vec{v}_c(\vec{k}) \times \vec{B} \right]$$

Take the cross product on both sides with the magnetic field:

$$\vec{B} \times \frac{d\hbar \vec{k}}{dt} = -e \vec{B} \times \left[ \vec{v}_c(\vec{k}) \times \vec{B} \right]$$

$$\vec{B} \times \frac{d\hbar \vec{k}}{dt} = -e \left[ \vec{v}_c(\vec{k}) - \vec{B} (\vec{B} \cdot \vec{v}_c(\vec{k})) \right]$$

$$\vec{B} \times \frac{d\hbar \vec{k}}{dt} = -e \left[ \frac{d\vec{r}(t)}{dt} |\vec{B}|^2 - \vec{B} \left( \vec{B} \cdot \frac{d\vec{r}(t)}{dt} \right) \right]$$

$$\text{Note: } \vec{A} \times (\vec{B} \times \vec{C}) = \vec{B} (\vec{A} \cdot \vec{C}) - \vec{C} (\vec{A} \cdot \vec{B})$$

$$\vec{B} \times \frac{d\hbar \vec{k}}{dt} = -e |\vec{B}|^2 \left[ \frac{d\vec{r}_{\perp}(t)}{dt} \right]$$

Now integrate both sides from time 0 to  $t$  to get:

$$\vec{r}_\perp(t) - \vec{r}_\perp(t=0) = -\frac{\hbar}{e|\vec{B}|^2} \vec{B} \times [\vec{k}(t) - \vec{k}(t=0)]$$

f) We have from lecture handouts:

$$M \cdot \frac{d\vec{v}_c(\vec{k})}{dt} = -e [\vec{v}_c(\vec{k}) \times \vec{B}_0 \hat{z}] = -e B_0 [\vec{v}_c(\vec{k}) \times \hat{z}]$$

$$\text{or: } \frac{d\vec{v}_c(\vec{k})}{dt} = -e B_0 M^{-1} \cdot [\vec{v}_c(\vec{k}) \times \hat{z}]$$

The above equation shows that the equations for the x- and y-components of the velocity depend only on the x- and y-components of the velocity – and not to the z-component of the velocity. Consequently, we can write the equations for only the x- and y-components as follows:

$$\frac{d}{dt} \begin{bmatrix} v_{cx} \\ v_{cy} \end{bmatrix} = -e B_0 \begin{bmatrix} 1/m_{xx} & 1/m_{xy} \\ 1/m_{yx} & 1/m_{yy} \end{bmatrix} \begin{bmatrix} v_{cy} \\ -v_{cx} \end{bmatrix}$$

We can now solve this simpler equation for the cyclotron frequency. The above are two coupled linear differential equations. One can take the derivative of the first and use the second to get a second order differential equation:

$$\begin{aligned} \frac{d^2 v_{cx}}{dt^2} &= -e^2 B_0^2 \left[ \frac{1}{m_{xx}} \frac{1}{m_{yy}} - \frac{1}{m_{xy}} \frac{1}{m_{yx}} \right] v_{cx} \\ &= -e^2 B_0^2 \left[ \frac{1}{m_{xx}} \frac{1}{m_{yy}} - \frac{1}{m_{xy}} \frac{1}{m_{yx}} \right] v_{cx} \end{aligned}$$

This implies the cyclotron frequency is:

$$\omega_c = \sqrt{e^2 B_0^2 \left[ \frac{1}{m_{xx}} \frac{1}{m_{yy}} - \frac{1}{m_{xy}} \frac{1}{m_{yx}} \right]}$$

The term in the square brackets is the determinant of the upper-left 2x2 submatrix of the inverse effective mass tensor.

$$\text{g) } \frac{1}{m_e} = \sqrt{\frac{1}{m_{xx}} \frac{1}{m_{yy}} - \frac{1}{m_{xy}} \frac{1}{m_{yx}}}$$

h) In spherical coordinates the unit vector  $\hat{n}$  can be written as,

$$\hat{n} = \sin \theta \cos \phi \hat{x} + \sin \theta \sin \phi \hat{y} + \cos \theta \hat{z}$$

If  $\hat{n}$  were in the  $\hat{z}$  direction, we would know the answer from part (f) above. So we perform a rotation of our coordinate system such that the z-axis of our rotated system is in the same direction as  $\hat{n}$ . This can be accomplished by a rotation matrix  $R$ :

$$R = \begin{bmatrix} \cos \phi \cos \theta & \sin \phi \cos \theta & -\sin \theta \\ -\sin \phi & \cos \phi & 0 \\ \cos \phi \sin \theta & \sin \phi \sin \theta & \cos \theta \end{bmatrix}$$

Note that, as wanted,  $R\hat{n} = \hat{z}$ . The inverse effective mass matrix in the new co-ordinate system would be,  $R.M^{-1}.R^{-1}$ . The square of the inverse cyclotron effective mass is, from part (f), given by the determinant of the upper 2x2 matrix of the matrix  $R.M^{-1}.R^{-1}$  and is as given in the homework set.

### Problem 6.5 (Effective masses and momentum operator matrix elements)

a) The solution requires just a little algebra. Note that both the first order perturbation term and the second order perturbation term both contain terms that are of second order in  $\Delta\bar{k}$ .

b) Again the final answer follows by a simple use of the general result in part (a) to the specific case. Since the mass matrix is isotropic and diagonal, one can work with the “xx” component of the inverse effective mass tensor to get:

$$\frac{1}{m_e} = \frac{1}{m} \left[ 1 + \frac{2}{m} \frac{\langle \psi_{c,\bar{k}=0} | \hat{P}_x | \psi_{v,\bar{k}=0} \rangle \langle \psi_{v,\bar{k}=0} | \hat{P}_x | \psi_{c,\bar{k}=0} \rangle}{E_g} \right]$$

$$-\frac{1}{m_h} = \frac{1}{m} \left[ 1 - \frac{2}{m} \frac{\langle \psi_{c,\bar{k}=0} | \hat{P}_x | \psi_{v,\bar{k}=0} \rangle \langle \psi_{v,\bar{k}=0} | \hat{P}_x | \psi_{c,\bar{k}=0} \rangle}{E_g} \right]$$

Subtraction of the above two equations gives the desired result.

### Problem 6.6 (Conductivity tensor of germanium)

For the pocket at  $(\pi/a, \pi/a, \pi/a)$  we have:

$$M^{-1} = \begin{bmatrix} 1/3m_\ell + 2/3m_t & 1/3m_\ell - 1/3m_t & 1/3m_\ell - 1/3m_t \\ 1/3m_\ell - 1/3m_t & 1/3m_\ell + 2/3m_t & 1/3m_\ell - 1/3m_t \\ 1/3m_\ell - 1/3m_t & 1/3m_\ell - 1/3m_t & 1/3m_\ell + 2/3m_t \end{bmatrix}$$

This pocket’s inverse effective mass tensor will serve as the reference. Now, for the pocket at  $(-\pi/a, -\pi/a, \pi/a)$  it was shown that:

$$M^{-1} = \begin{bmatrix} 1/3m_\ell + 2/3m_t & 1/3m_\ell - 1/3m_t & -(1/3m_\ell - 1/3m_t) \\ 1/3m_\ell - 1/3m_t & 1/3m_\ell + 2/3m_t & -(1/3m_\ell - 1/3m_t) \\ -(1/3m_\ell - 1/3m_t) & -(1/3m_\ell - 1/3m_t) & 1/3m_\ell + 2/3m_t \end{bmatrix}$$

Now we look at the pocket at  $(-\pi/a, \pi/a, \pi/a)$ . If we let  $E_x$  become  $-E_x$  then in the current density contributed from the pocket at  $(-\pi/a, \pi/a, \pi/a)$  we should see  $J_x$  become  $-J_x$  and  $J_y$  and  $J_z$  should remain the same. This can only happen if the inverse mass tensor for the pocket at  $(-\pi/a, \pi/a, \pi/a)$  is,

$$M^{-1} = \begin{bmatrix} 1/3m_\ell + 2/3m_t & -(1/3m_\ell - 1/3m_t) & -(1/3m_\ell - 1/3m_t) \\ -(1/3m_\ell - 1/3m_t) & 1/3m_\ell + 2/3m_t & 1/3m_\ell - 1/3m_t \\ -(1/3m_\ell - 1/3m_t) & 1/3m_\ell - 1/3m_t & 1/3m_\ell + 2/3m_t \end{bmatrix}$$

Now we look at the pocket at  $(\pi/a, -\pi/a, \pi/a)$ . If we let  $E_y$  become  $-E_y$  then in the current density contributed from the pocket at  $(\pi/a, -\pi/a, \pi/a)$  we should see  $J_y$  become  $-J_y$  and  $J_x$  and  $J_z$  should remain the same. This can only happen if the inverse mass tensor for the pocket at  $(\pi/a, -\pi/a, \pi/a)$  is,

$$M^{-1} = \begin{bmatrix} 1/3m_\ell + 2/3m_t & -(1/3m_\ell - 1/3m_t) & 1/3m_\ell - 1/3m_t \\ -(1/3m_\ell - 1/3m_t) & 1/3m_\ell + 2/3m_t & -(1/3m_\ell - 1/3m_t) \\ 1/3m_\ell - 1/3m_t & -(1/3m_\ell - 1/3m_t) & 1/3m_\ell + 2/3m_t \end{bmatrix}$$

Now we add contributions from all pockets to get the expression for the total current density:

$$\begin{bmatrix} J_x \\ J_y \\ J_z \end{bmatrix} = \bar{\bar{\sigma}} \cdot \begin{bmatrix} E_x \\ E_y \\ E_z \end{bmatrix}$$

$$\bar{\bar{\sigma}} = n e^2 \tau \begin{bmatrix} 1/3 m_\ell + 2/3 m_t & 0 & 0 \\ 0 & 1/3 m_\ell + 2/3 m_t & 0 \\ 0 & 0 & 1/3 m_\ell + 2/3 m_t \end{bmatrix}$$

Conductivity tensor is diagonal and isotropic!! This is the case for all materials with cubic symmetry (which includes FCC, BCC, SC).