Departments of ECE and MSE, Cornell University

ECE 4070/MSE 5470: Physics of Semiconductor and Nanostructures

Spring 2015

Homework 7: Solutions **Due on April 20, 2015 at 5:00 PM**

Problem 7.1 (The deep-acceptor problem and the 2014 Physics Nobel Prize)

```
q = 1.6*10^-19            (* Electron charge, Coulomb *)
hbar = 6.63/(2π) * 10^-34 (* Reduced Planck's constant, J.s *)
kb = 1.38*10^-23          (* Boltzmann constant, J/K *)
m0 = 9.1*10^-31           (* Electron rest mass, Kg *)
meGaN = 0.2*m0            (* Electron effective mass, CB *)
mhGaN = 1.4*m0            (* Hole effective mass, VB *)
Nc[T_] = 2*((meGaN*kb*T)/(2*π*hbar^2))^(3/2) * 10^-6   (* CB edge Effective DOS, cm^-3 *)
Nv[T_] = 2*((mhGaN*kb*T)/(2*π*hbar^2))^(3/2) * 10^-6   (* VB edge Effective DOS, cm^-3 *)
F[η_] = Abs[2/Sqrt[π] Integrate[Sqrt[x]/(1 + Exp[x - η]), {x, 0, ∞}]]
(* Fermi-Dirac Integral of order j=1/2 *)
```

```
(* In energy scale, Ev is set to zero, and Ec=Ev+Eg=3.4 eV. Ef is in eV too! *)
Eg = 3.4          (* Bandgap of GaN, eV.  Also conduction band edge!*)
Ea = 0.16         (* Acceptor ionization energy, eV *)
Ed = Eg - 0.01    (* Donor activation energy, eV *)
ND = 10^14        (* Donor atom volume density, cm^-3 *)
NA = 10^18        (* Acceptor atom volume density, cm^-3 *)
```

```
NDp[Ef_, T_] = ND/(1 + 2*Exp[(q*(Ef - Ed))/(kb*T)])   (* Ionized donor density, cm^-3 *)
NAm[Ef_, T_] = NA/(1 + 4*Exp[(q*(Ea - Ef))/(kb*T)])   (* Ionized acceptor density, cm^-3 *)
n[Ef_, T_] = Nc[T]*F[(q*(Ef - Eg))/(kb*T)]   (* Free electron density in cm^-3 dependent on Ef *)
p[Ef_, T_] = Nv[T]*F[(q*(0 - Ef))/(kb*T)]    (* Free hole density in cm^-3 dependent on Ef *)
```

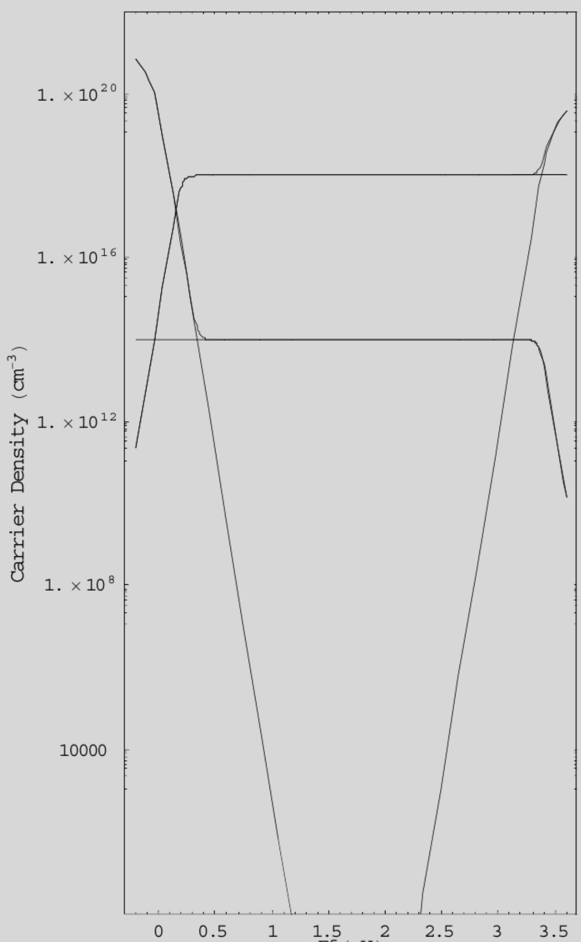
```
(* Numerical Solution of the charge-
  neutrality equation gives us the Fermi Level in eV.  Note that you can do this
   for any general temperature and doping densities. *)
FindRoot[NDp[Ef, 300] + p[Ef, 300] - (NAm[Ef, 300] + n[Ef, 300]) == 0, {Ef, 0}]
```

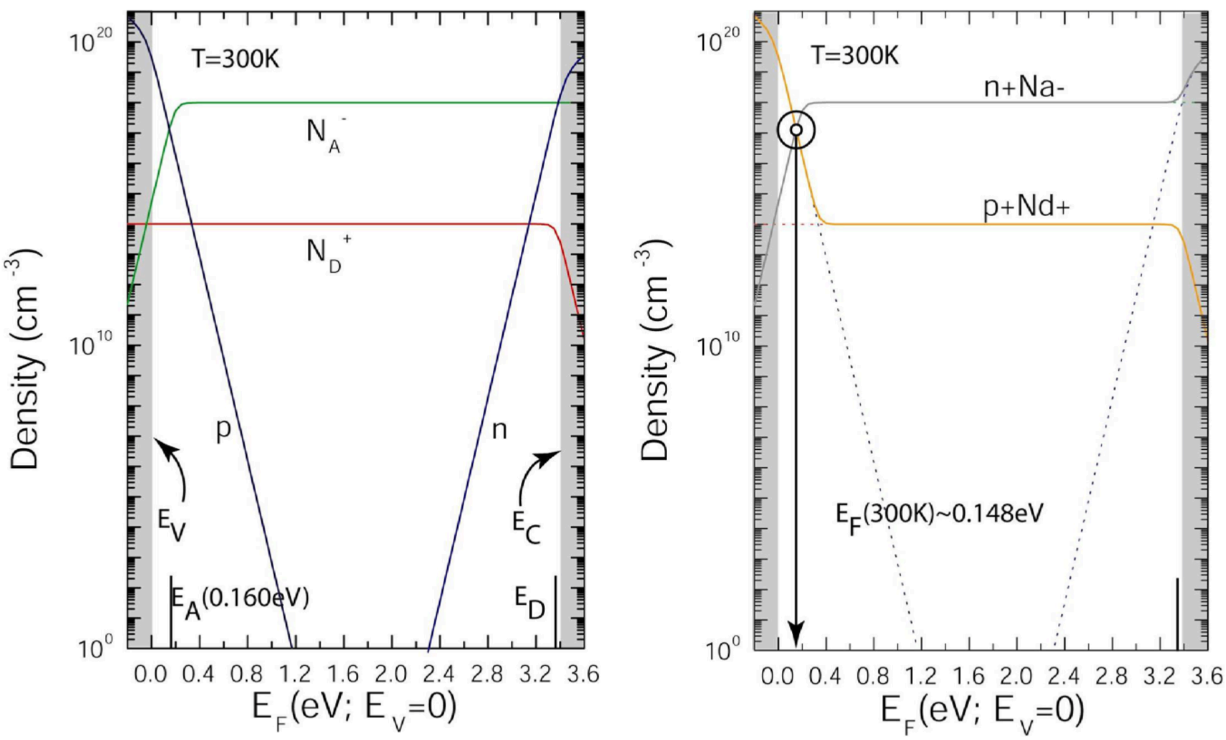
```
{Ef → 0.147989}
```

```
p[0.147989, 300]
(* This is the Hole concentration, the semiconductor is obviously p-type *)
```

1.35713×10^{17}

```
(*----You can do a Graphical Solution also - See the attached figures,
 which are basically the plot below labeled and suitably commented upon----*)
LogPlot[{NDp[Ef, 300], NAm[Ef, 300], n[Ef, 300], p[Ef, 300], NDp[Ef, 300] + p[Ef, 300]
  NAm[Ef, 300] + n[Ef, 300]}, {Ef, -0.2, 3.6}, PlotRange → {10^0, 10^22}, Frame → True,
 AspectRatio → 2, FrameLabel → {"Ef(eV)", "Carrier Density (cm^-3)"}]
```




T=300K
N_A^-
N_D^+
p
n
E_V
E_C
E_A(0.160eV)
E_D
Density (cm^{-3})
E_F(eV; E_V=0)
T=300K
n+Na-
p+Nd+
E_F(300K)~0.148eV
Density (cm^{-3})
E_F(eV; E_V=0)

Problem 7.2 (Time-dependent Effective Mass Equation)

a) The answer is,

$$\phi(\vec{r},t) = \exp\left[-\frac{i}{\hbar} \int_0^t \left(E(t') + e\vec{E}\,.\,\vec{r} \right) dt' \right]$$

The solution can be checked by direct substitution is the effective mass equation,

$$\left[E_n\left(\vec{k}_o - i\nabla\right) + e\vec{E}.\,\vec{r} \right] \phi(\vec{r},t) = i\hbar \frac{\partial \phi(\vec{r},t)}{\partial t}$$

b) Upon substitution in the effective mass equation, the assumed solution gives,

$$E(t) = E_n\left(\vec{k}_o - \frac{e\vec{E}}{\hbar} t \right)$$

Therefore, the energy of the solution is time dependent and changes with time as the wavevector (or the crystal momentum) changes.

Problem 7.3 (Probability currents for the Effective Mass equation)

a) Note that irrespective of the details of the energy band dispersion relation, a plane wave is always an eigenfunction of the $E_n\left(\vec{k}_o - i\nabla\right)$ operator,

$$E_n\left(\vec{k}_o - i\nabla\right)\phi(\vec{r},t) = E_n\left(\vec{k}_o - i\nabla\right) e^{i\vec{q}.\vec{r}} = \sum_j E_n\left(\vec{R}_j\right) e^{i\left(\vec{k}_o - i\nabla\right)\vec{R}_j} e^{i\vec{q}.\vec{r}}$$

$$= \sum_j E_n\left(\vec{R}_j\right) e^{i\vec{k}_o.\vec{R}_j} e^{i\vec{q}.\left(\vec{r}+\vec{R}_j\right)} = E_n\left(\vec{k}_o + \vec{q}\right) e^{i\vec{q}.\vec{r}}$$

So a plane wave has to satisfy the equation,

$$\left[\hat{E}_c\left(\vec{k}_o - i\nabla\right) \right] \phi(\vec{r}) = E\,\phi(\vec{r})$$

with energy eigenvalue equal to $E_c\left(\vec{k}_o + \vec{q}\right)$, which equals,

$$E_c + \frac{\hbar^2 (q_x)^2}{2m_x} + \frac{\hbar^2 \left(q_y\right)^2}{2m_y} + \frac{\hbar^2 (q_z)^2}{2m_z}$$

b) $$\psi(\vec{r}) = \phi(\vec{r})\,\psi_{c,\vec{k}_o}(\vec{r}) = e^{i\vec{q}.\vec{r}}\,\psi_{c,\vec{k}_o}(\vec{r})$$

$$\Rightarrow \psi\left(\vec{r}+\vec{R}\right) = \phi\left(\vec{r}+\vec{R}\right)\psi_{c,\vec{k}_o}\left(\vec{r}+\vec{R}\right) = e^{i\left(\vec{k}_o+\vec{q}\right)\vec{r}}\,\phi(\vec{r})\,\psi_{c,\vec{k}_o}(\vec{r})$$

c) $$J_\alpha(\vec{r}) = \sum_\beta \phi^*(\vec{r}) \frac{\hbar}{2im_{\alpha\beta}} \partial_\beta \phi(\vec{r}) + c.c.$$

$$\Rightarrow J_x(\vec{r}) = \phi^*(\vec{r}) \frac{\hbar}{2im_x} \partial_x \phi(\vec{r}) + c.c = \frac{\hbar q_x}{m_x}$$

$$\Rightarrow J_y(\vec{r}) = \phi^*(\vec{r}) \frac{\hbar}{2im_y} \partial_y \phi(\vec{r}) + c.c = \frac{\hbar q_y}{m_y}$$

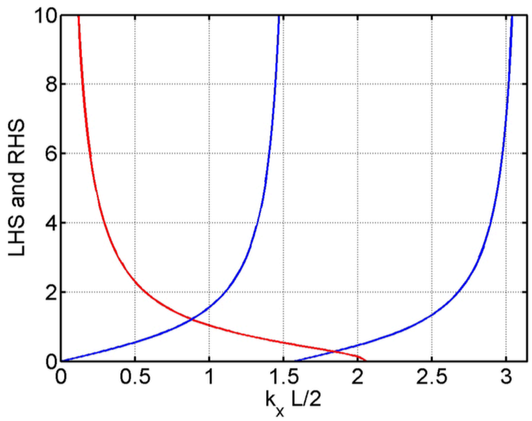
$$\Rightarrow J_z(\vec{r}) = \phi^*(\vec{r}) \frac{\hbar}{2im_z} \partial_z \phi(\vec{r}) + c.c = \frac{\hbar q_z}{m_z}$$

Problem 7.4 (A Quantum Well in a Semiconductor Heterostructure)

a) The transcendental equation to be solved are:

$$\begin{cases} \tan\left(\dfrac{k_x L}{2}\right) = \dfrac{m_{x1}}{m_{x2}} \dfrac{\alpha}{k_x} = \dfrac{m_{x1}}{m_{x2}} \dfrac{\sqrt{\dfrac{2m_{x2}}{\hbar^2}\Delta E_c - \dfrac{m_{x2}}{m1} k_x^2}}{k_x} \\ -\cot\left(\dfrac{k_x L}{2}\right) = \dfrac{m_{x1}}{m_{x2}} \dfrac{\alpha}{k_x} = \dfrac{m_{x1}}{m_{x2}} \dfrac{\sqrt{\dfrac{2m_{x2}}{\hbar^2}\Delta E_c - \dfrac{m_{x2}}{m_{x1}} k_x^2}}{k_x} \end{cases}$$

These are slightly modified from the ones in the lecture handouts because the effective masses in the x-direction in the well and the barrier regions are different. We calculate the value of k_x for which the RHS goes to zero. This comes out to be, $k_x L/2 = 2.05$. This is bigger than $\pi/2$ but smaller than π so there are two bound states.



b) The RHS and the LHS of the transcendental equations are plotted. The intersections give the quantized values of k_x. The corresponding energies are:

$E_1 = 27.7$ meV

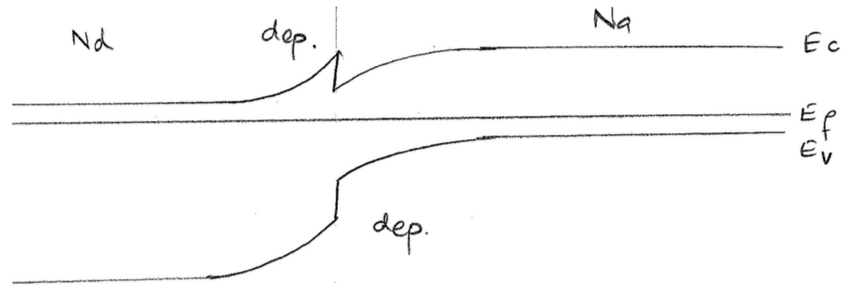
$E_2 = 121.3$ meV

c) $$n = \frac{\sqrt{m_y m_z}}{\pi \hbar^2} KT \log\left(1 + e^{(E_f - E_1 - E_{c1})/KT}\right) + \frac{\sqrt{m_y m_z}}{\pi \hbar^2} KT \log\left(1 + e^{(E_f - E_2 - E_{c1})/KT}\right)$$

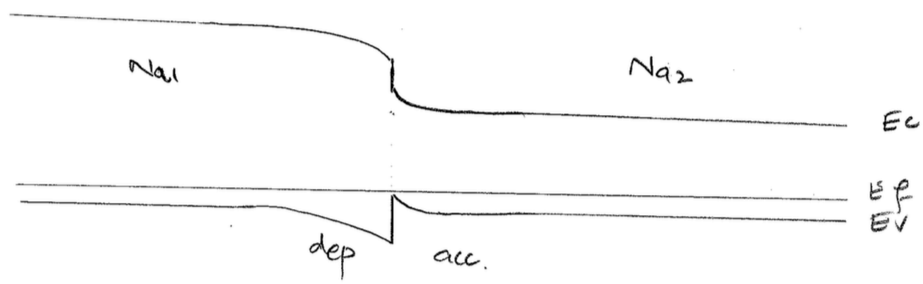
d) Assume T=300K (room temperature). Plot the RHS as a function of the Fermi level and see which value of the Fermi level gives you the electron density on the LHS. This method yields $E_f - E_{c1} = 53.4$ meV.

Problem 7.5 (Equilibrium in Semiconductor Heterojunctions with various band offsets)

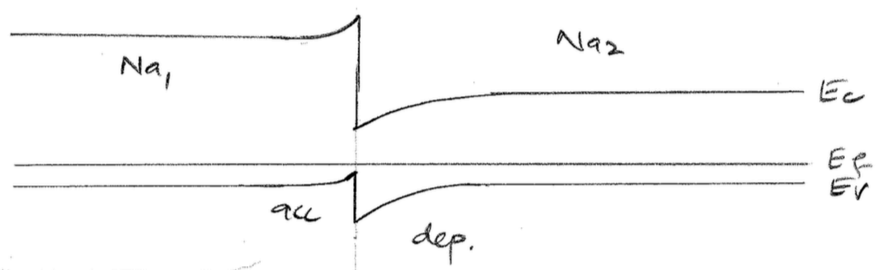
a)



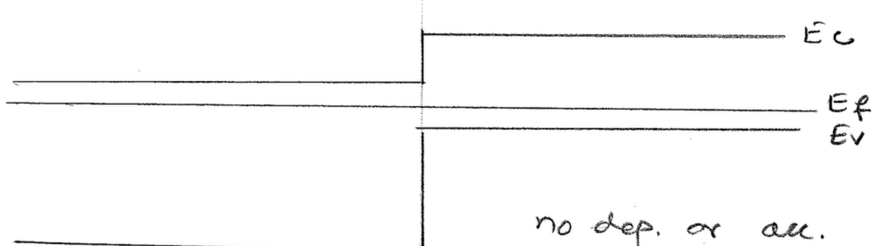
b)



c)



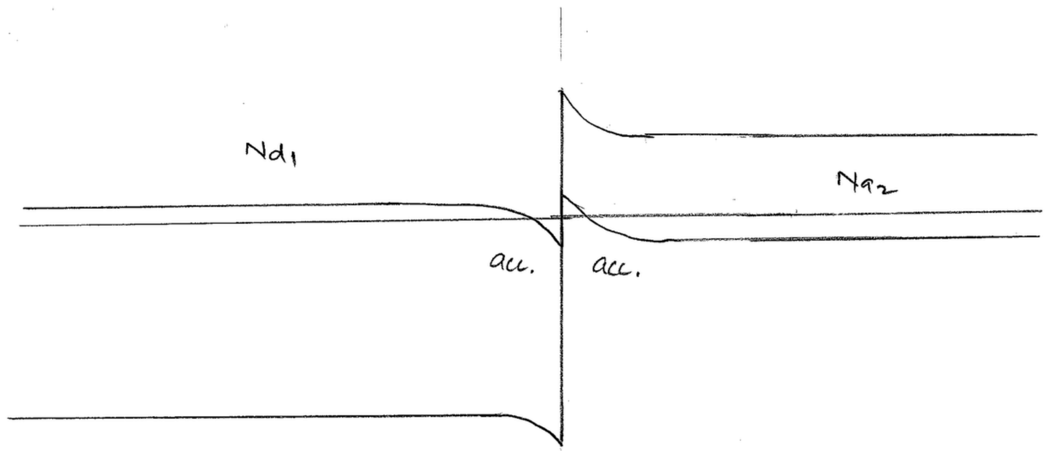
d) Fermi levels already aligned.



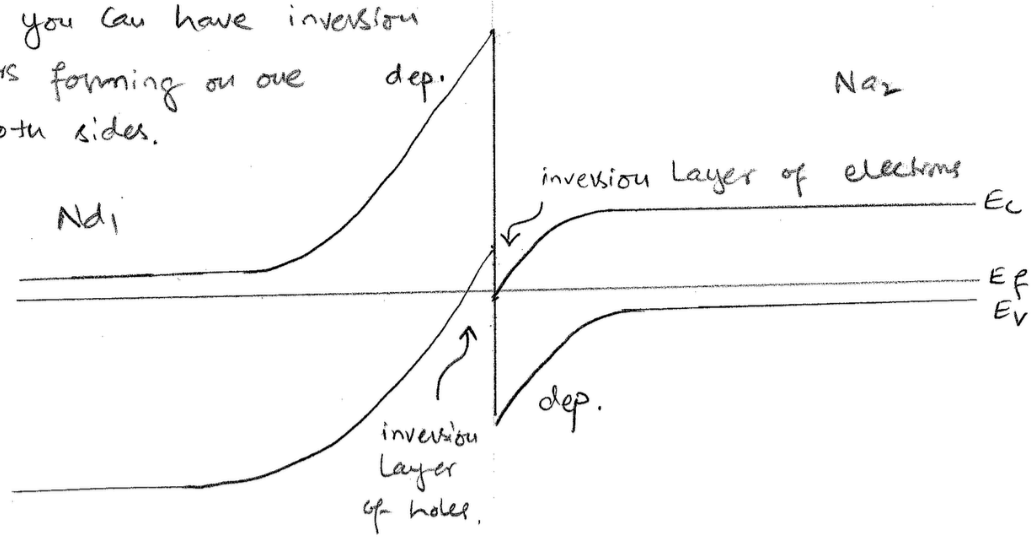
no dep. or acc. regions.

$V_{bi} = 0$.

e)



f) Here you can have inversion Layers forming on one or both sides.



Problem 7.6 (Bloch transport and Bloch Oscillations)

a) See next page. The easy way to find constant-energy contours $E(k_x, k_y) = 0, \pm E_0$ is to see the values attained at the axes $(k_x, 0)$ + $(0, k_y)$ + following the contours.

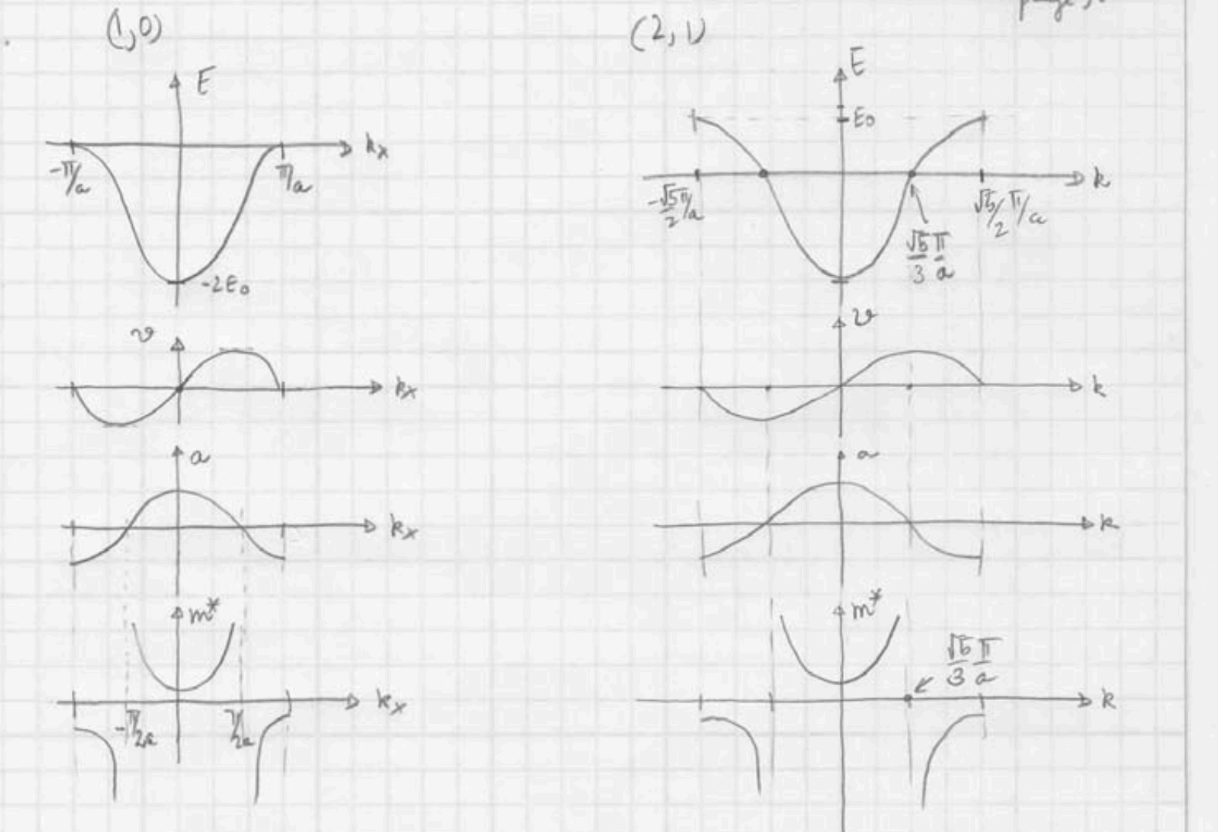
b) In the $(1,0)$ direction,

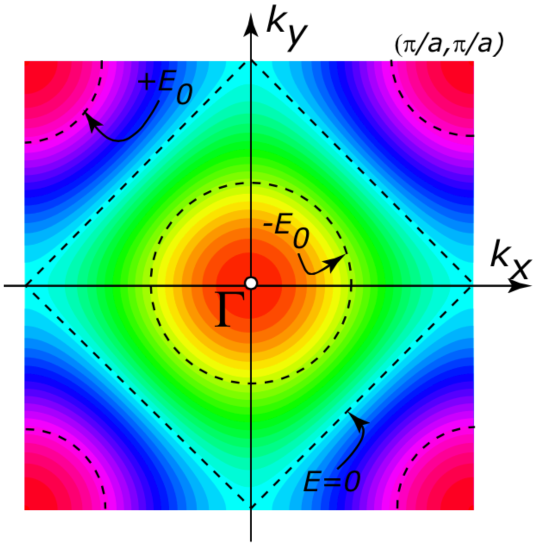
$$E(k_x, 0) = -E_0\left[\cos k_x a + 1\right] \rightarrow \text{from } 0 \text{ to } -2E_0.$$

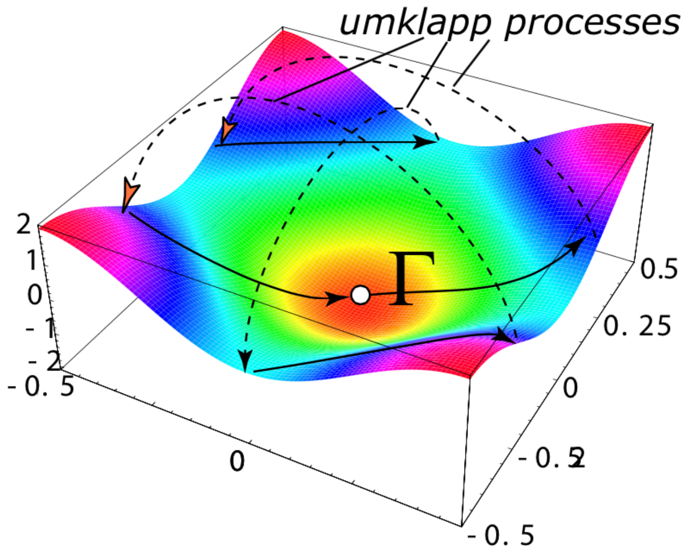
In the $(2,1)$ direction,

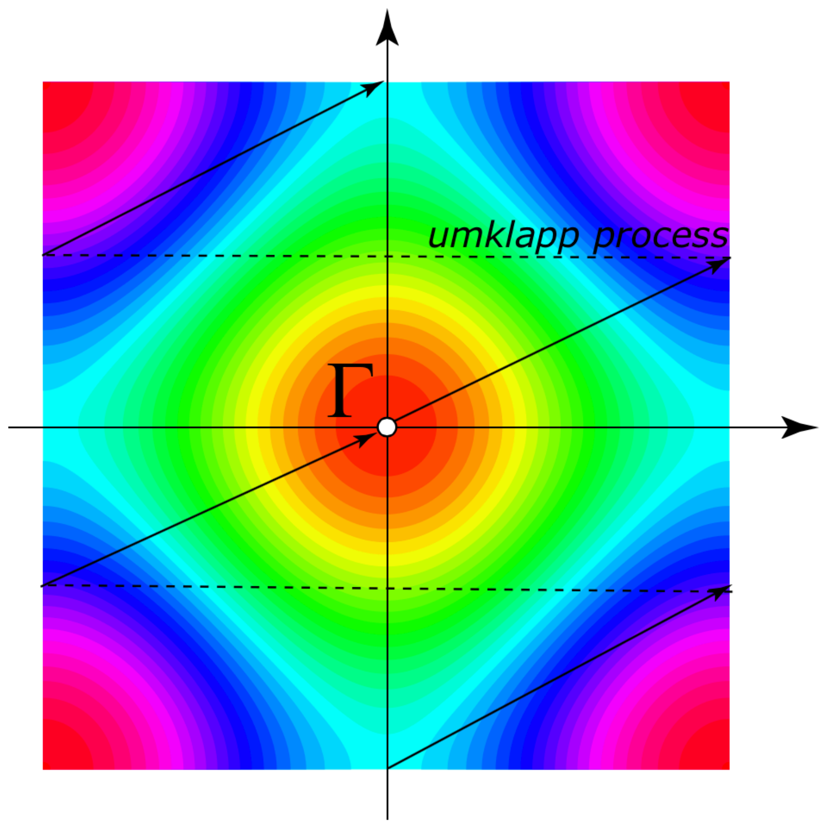
$$E(k_x, k_y) = -E_0\left[\cos k_x a + \cos k_y a\right] \rightarrow \text{from } -2E_0 \text{ to } +E_0$$

(see contours on next page).





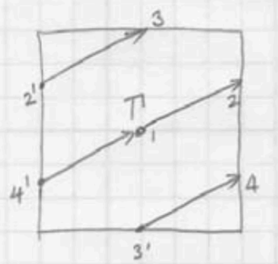




Electron trajectory in the BZ
(Bloch Oscillations)

Part c:

The trajectory is shown in the previous page. The force will cause the electron to move in the same direction, across constant energy surfaces. At the BZ edges, the electron suffers Umklapp scattering to enter the BZ from the other end. The motion is



$$1 \to \underbrace{2 \to 2'}_{\text{Umklapp}} \to \underbrace{3 \to 3'}_{\text{umklapp}} \to \underbrace{4 \to 4'}_{\text{umklapp}} \to 1$$

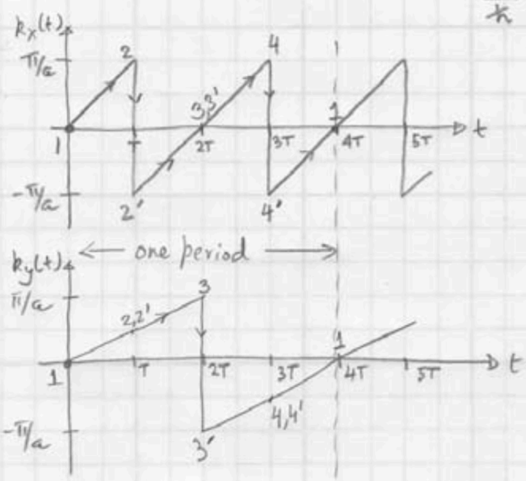
$\vec{F} = \hbar \dfrac{d\vec{k}}{dt}$.

$\Delta \vec{k} = \vec{G} = \left(-\dfrac{2\pi}{a}, 0\right)$ $\qquad \Delta \vec{k} = \left(0, -\dfrac{2\pi}{a}\right)$ $\qquad \Delta \vec{k} = \left(-\dfrac{2\pi}{a}, 0\right)$

$$F_x = \hbar \frac{dk_x}{dt} \quad \Rightarrow \quad k_x(t) = k_x(0) + \frac{F_x}{\hbar} t$$

Time taken from $1 \to 2$ is given by

$$\frac{F_x}{\hbar}\tau = \pi/a \quad \Rightarrow \quad \tau = \frac{\pi \hbar}{a F_x} = T \, !$$



Both $k_x(t)$ & $k_y(t)$ "oscillate" with different periods. However, the particle oscillates in k-space with a period 4T.

Parts d, e:

To find the real-space trajectories, we note that

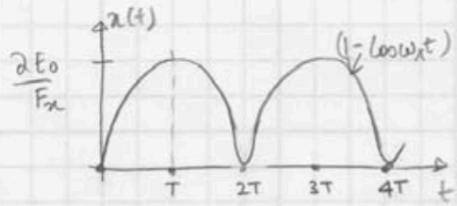
$$k_x(t) = \frac{F_x}{\hbar} t \qquad k_y(t) = \frac{F_x}{2\hbar} t$$

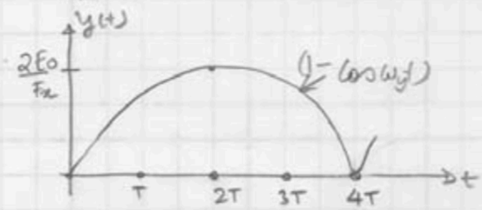
$$v_x(t) = \frac{1}{\hbar}\frac{\partial E(k_x, k_y)}{\partial k_x} = \frac{a E_0}{\hbar} \sin k_x(t) a = \frac{a E_0}{\hbar} \sin\Big(\underbrace{\frac{F_x a}{\hbar}}_{\omega_x = \frac{F_x a}{\hbar}} t\Big) = \frac{a E_0}{\hbar} \sin \omega_x t$$

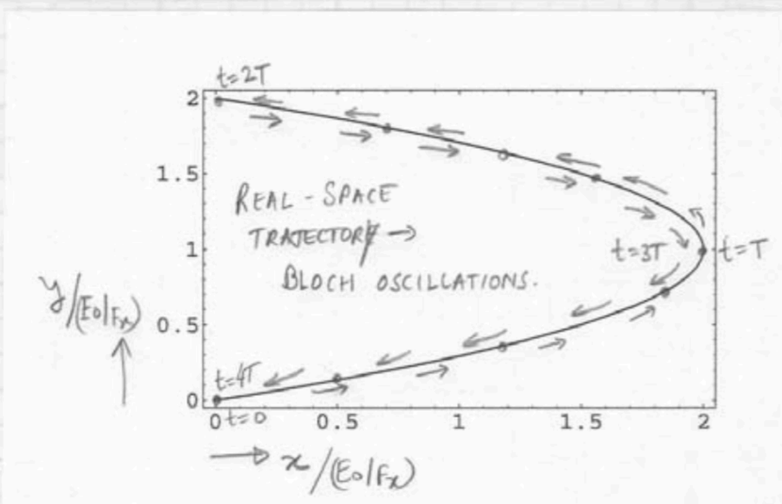
$$v_y(t) = \frac{1}{\hbar}\frac{\partial E(k_x, k_y)}{\partial k_y} = \frac{a E_0}{\hbar} \sin(\omega_y t) \qquad \left(\omega_y = \frac{F_y a}{\hbar} = \frac{\omega_x}{2}\right)$$

$$\Rightarrow \quad x(t) = \int_0^t dt' \, v_x(t') = \frac{E_0}{F_x}\Big[\overbrace{1 - \cos(\omega_x t)}^{\text{max: } 2}\Big] \leftarrow \text{always +ve}$$

$$y(t) = \int_0^t dt' \, v_y(t') = \frac{E_0}{F_x}\left[1 - \cos \omega_y t\right] \leftarrow \text{always +ve.}$$







Part f:

Bloch oscillations: Attempts to mitigate the effect of scattering to observe BO^s have led to investigation of superlattices, with artificial periodicity $L = \underset{\text{SL period}}{n}\,\underset{\text{lattice constant}}{a}$, which leads to a BZ edge at

$$k = \frac{2\pi}{na} = \text{'}\frac{1}{n}\text{'} \text{ times smaller than the crystal BZ.}$$

Various approaches are feasible – other than the superlattice approach mentioned here!