ECE 656 Homework SOLUTIONS (Week 11)

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1) Consider a semiconductor with a slowly varying effective mass, $m^*(x)$. Derive the equation of motion for an electron in *k*-space analogous to the result for a constant effective mass:

$$\frac{d(\hbar k_x)}{dt} = F_e = -\frac{dE_C(x)}{dx}.$$

Solution:

$$E_{TOT} = E = E_C(x) + E(k,x) = E_C(x) + \frac{\hbar^2 k^2}{2m^*(x)} \qquad \text{(i)}$$

$$\frac{dE}{dt} = 0 = \frac{dE_C}{dx}\frac{dx}{dt} + \frac{\hbar^2 k^2}{2}\frac{d}{dx}\left(\frac{1}{m^*(x)}\right)\frac{dx}{dt} + \frac{1}{\hbar}\frac{dE(k,x)}{dk}\frac{d(\hbar k)}{dt} \qquad \text{(ii)}$$

Recognizing that

$$\frac{dx}{dt} = \upsilon_x = \frac{1}{\hbar}\frac{dE(k,x)}{dk} \qquad \text{(iii)}$$

(ii) becomes

$$\frac{d(\hbar k)}{dt} = -\frac{dE_C}{dx} - \frac{\hbar^2 k^2}{2m^*}\left\{m^* \frac{d}{dx}\left(\frac{1}{m^*(x)}\right)\right\} \qquad \text{(iv)}$$

or

$$\boxed{\frac{d(\hbar k)}{dt} = -\frac{dE_C}{dx} + \frac{\hbar^2 k^2}{2m^*}\left(\frac{1}{m^*}\frac{dm^*}{dx}\right)}$$

2) Consider a semiconductor with a position dependent effective mass and electron affinity, $\chi(x)$, so that

$$E_C(x) = E_{vac} - \chi(x) - qV(x),$$

where E_{vac} is a constant, reference energy (the vacuum level) and $V(x)$ is the electrostatic potential.

ECE 656 Homework Solutions (Week 11) (continued)

Solve the steady-state BTE in the relaxation time approximation and compare your result to the results for a constant effective mass and electron affinity:

$$J_{nx} = \sigma \frac{d\left(F_n/q\right)}{dx} - \sigma S \frac{dT}{dx}$$

Solution:

$$\frac{\partial f}{\partial t} + \upsilon_x \frac{\partial f}{\partial x} + \frac{d\left(\hbar k\right)}{dt}\frac{\partial f}{\partial p_x} = -\frac{\delta f}{\tau_m} \qquad \text{(i)}$$

Use the result from prob. 1):

$$\frac{d\left(\hbar k\right)}{dt} = -\frac{dE_C}{dx} + \frac{\hbar^2 k^2}{2m^*}\left(\frac{1}{m^*}\frac{dm^*}{dx}\right) \qquad \text{(ii)}$$

and assuming steady-state conditions, (i) becomes

$$\upsilon_x \frac{\partial f}{\partial x} + \left\{-\frac{dE_C}{dx} + \frac{\hbar^2 k^2}{2m^*}\left(\frac{1}{m^*}\frac{dm^*}{dx}\right)\right\}\frac{\partial f}{\partial p_x} = -\frac{\delta f}{\tau_m} \qquad \text{(iii)}$$

Replacing f by f_0 on the LHS:

$$\delta f = -\tau_m \upsilon_x \frac{\partial f_0}{\partial x} + \tau_m \left\{\frac{dE_C}{dx} - \frac{\hbar^2 k^2}{2m^*}\left(\frac{1}{m^*}\frac{dm^*}{dx}\right)\right\}\frac{\partial f_0}{\partial p_x} \qquad \text{(iv)}$$

$$f_0 = \frac{1}{1+e^{\Theta}} \qquad \Theta = \left[E_C\left(x\right) + E\left(k,x\right) - F_n\left(x\right)\right]/k_B T \qquad \text{(v)}$$

$$\frac{\partial f_0}{\partial x} = \frac{\partial f_0}{\partial \Theta}\frac{\partial \Theta}{\partial x} = k_B T \frac{\partial f_0}{\partial E}\frac{\partial \Theta}{\partial x} \qquad \text{(vi)}$$

$$\frac{\partial \Theta}{\partial x} = \frac{\partial}{\partial x}\left\{\left[E_C\left(x\right) + E\left(k,x\right) - F_n\left(x\right)\right]/k_B T\right\} \qquad \text{(vii)}$$

$$\frac{\partial \Theta}{\partial x} = \frac{1}{k_B T}\left[\frac{\partial E_C\left(x\right)}{\partial x} - \frac{\hbar^2 k^2}{2}\frac{1}{\left(m^*\right)^2}\frac{dm^*}{dx} - \frac{dF_n}{dx}\right] + \left[E_C\left(x\right) + E\left(k,x\right) - F_n\left(x\right)\right]\frac{1}{k_B}\frac{d}{dx}\left(\frac{1}{T}\right) \qquad \text{(viii)}$$

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Using (vii) in (vi), we find

$$\frac{\partial f_0}{\partial x} = \frac{\partial f_0}{\partial E}\left\{ \begin{array}{l} \left[\dfrac{\partial E_C(x)}{\partial x} - E(k,x)\left(\dfrac{1}{m^*}\dfrac{dm^*}{dx}\right) - \dfrac{dF_n}{dx} \right] \\ +T\left[E_C(x) + E(k,x) - F_n(x) \right]\dfrac{d}{dx}\left(\dfrac{1}{T}\right) \end{array} \right\} \qquad \text{(ix)}$$

Now consider the derivative in momentum space:

$$\frac{\partial f_0}{\partial p_x} = \frac{\partial f_0}{\partial \Theta}\frac{\partial \Theta}{\partial p_x} = k_B T \frac{\partial f_0}{\partial E}\frac{\partial \Theta}{\partial p_x} \qquad \text{(x)}$$

$$\frac{\partial \Theta}{\partial p_x} = \upsilon_x / (k_B T) \qquad \text{(xi)}$$

so (x) becomes

$$\frac{\partial f_0}{\partial p_x} = \frac{\partial f_0}{\partial E}\upsilon_x \qquad \text{(xii)}$$

Using (ix) and (xii) in (iv), we write the solution to the BTE as

$$\delta f = -\tau_m \upsilon_x \frac{\partial f_0}{\partial x} + \tau_m \left\{ \frac{dE_C}{dx} - E(k,x)\left(\frac{1}{m^*}\frac{dm^*}{dx}\right)\right\}\frac{\partial f_0}{\partial p_x} \qquad \text{(xiii)}$$

After simplifying the algebra, the final result:

$$\boxed{\delta f = -\tau_m\left(-\frac{\partial f_0}{\partial E}\right)\upsilon_x\left\{-\frac{dF_n}{dx} + T\left[E_C(x) + E(k,x) - F_n(x)\right]\frac{d}{dx}\left(\frac{1}{T}\right)\right\}}$$

is **exactly the same as the result for a position-independent bandtructure.** Accordingly, the current equation for a semiconductor with a position-dependent bandstructure is identical to that of a uniform semiconductor:

$$J_{nx} = \sigma \frac{d(F_n/q)}{dx} - \sigma S \frac{dT}{dx}$$

ECE 656 Homework Solutions (Week 11) (continued)

3) Solve the steady-state BTE in the Relaxation Time Approximation and derive an expression for the transport tensor, $[\kappa_0]_{ij}$ in the absence of a B-field.

Solution:

The heat current is

$$J_{Qi} = \frac{1}{\Omega}\sum_{\vec{k}}\left(E - F_n\right)\upsilon_i \delta f \qquad \text{(i)}$$

Note that E is the total energy,

$$E = E_C\left(\vec{r}\right) + E\left(\vec{k}\right) \qquad \text{(ii)}$$

The solution to the BTE is:

$$\delta f = \tau_m\left(-\frac{\partial f_0}{\partial E}\right)\upsilon_j \mathcal{F}_j \qquad \text{(iii)}$$

where the generalized force is:

$$\mathcal{F}_j = -\partial_j F_n - \left[E_C\left(\vec{r}\right) + E\left(\vec{k},\vec{r}\right) - F_n\left(\vec{r}\right)\right]\frac{1}{T}\partial_j T$$

$$= -\partial_j F_n - \left[E - F_n\left(\vec{r}\right)\right]\frac{1}{T}\partial_j T \qquad \text{(iv)}$$

Using (ii) and (iii), (i) becomes

$$J_{Qi} = \frac{1}{\Omega}\sum_{\vec{k}}\tau_m\left(-\frac{\partial f_0}{\partial E}\right)\upsilon_i\upsilon_j\left(E - F_n\right)\left\{-\partial_j F_n - \left[E - F_n\left(\vec{r}\right)\right]\frac{1}{T}\partial_j T\right\} \qquad \text{(v)}$$

The second term in curly brackets gives the thermal conductivity.

$$\boxed{\left.\kappa_0\right)_{i,j} = \frac{1}{\Omega}\sum_{\vec{k}}\tau_m \frac{\upsilon_i\upsilon_j\left(E - F_n\right)^2}{T}\left(-\frac{\partial f_0}{\partial E}\right)}$$