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:

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

$$\frac{dE}{dt} = 0 = \frac{dE_C}{dx} \frac{dt}{dx} + \frac{\hbar^2}{2} \frac{k_x^2}{m^*(x)} \frac{dx}{dt} + \frac{1}{\hbar} \frac{dE(k,x)}{dk} \frac{dk}{dt} \quad (ii)$$

Recognizing that

$$\frac{dx}{dt} = v^* = \frac{1}{\hbar} \frac{dE(k,x)}{dk} \quad (iii)$$

(ii) becomes

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

or

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

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

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

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

\[ J_{\text{ex}} = \sigma \frac{d(F_n/q)}{dx} - \sigma S \frac{dT}{dx} \]

**Solution:**

\[ \frac{\partial f}{\partial t} + v_x \frac{\partial f}{\partial x} + \frac{d(hk)}{dt} \frac{\partial f}{\partial p_x} = -\frac{\delta f}{\tau_m} \]  

(i)

Use the result from prob. 1):

\[ \frac{d(hk)}{dt} = -\frac{dE_C}{dx} + \frac{h^2k^2}{2m^*} \left( \frac{1}{m^*} \frac{dm^*}{dx} \right) \]  

(ii)

and assuming steady-state conditions, (i) becomes

\[ v_x \frac{\partial f}{\partial x} + \left\{ -\frac{dE_C}{dx} + \frac{h^2k^2}{2m^*} \left( \frac{1}{m^*} \frac{dm^*}{dx} \right) \right\} \frac{\partial f}{\partial p_x} = -\frac{\delta f}{\tau_m} \]  

(iii)

Replacing \( f \) by \( f_0 \) on the LHS:

\[ \delta f = -\tau_n v_x \frac{\partial f_0}{\partial x} + \tau_m \left\{ -\frac{dE_C}{dx} + \frac{h^2k^2}{2m^*} \left( \frac{1}{m^*} \frac{dm^*}{dx} \right) \right\} \frac{\partial f_0}{\partial p_x} \]  

(iv)

\[ f_0 = \frac{1}{1 + e^{\Theta}} \quad \Theta = \left[ E_C(x) + E(k,x) - F_n(x) \right] / k_T \]  

(v)

\[ \frac{\partial f_0}{\partial x} = \frac{\partial f_0}{\partial \Theta} \frac{\partial \Theta}{\partial x} = k_T \frac{\partial f_0}{\partial E} \frac{\partial E}{\partial x} \]  

(vi)

\[ \frac{\partial \Theta}{\partial x} = \frac{\partial}{\partial x} \left\{ \left[ E_C(x) + E(k,x) - F_n(x) \right] / k_T \right\} \]  

(vii)

\[ \frac{\partial \Theta}{\partial x} = \frac{1}{k_T} \left[ \frac{\partial E_C(x)}{\partial x} - \frac{h^2k^2}{2} \frac{1}{m^*} \frac{dm^*}{dx} \frac{dF_n}{dx} \right] \]  

\[ + \left[ E_C(x) + E(k,x) - F_n(x) \right] \frac{1}{k_T} \frac{d}{dx} \frac{1}{T} \]  

(viii)
Using (vii) in (vi), we find
\[ \frac{\partial f_0}{\partial x} = \frac{\partial f_0}{\partial E} \left[ \frac{\partial E_C(x)}{\partial x} - E(k, x) \left( \frac{1}{m^*} \frac{dm^*}{dx} \right) - \frac{d F_n}{dx} \right] \]
\[ + T \left[ E_C(x) + E(k, x) - F_n(x) \right] \frac{d}{dx} \left( \frac{1}{T} \right) \]  

(ix)

Now consider the derivative in momentum space:
\[ \frac{\partial f_0}{\partial p_x} = \frac{\partial f_0}{\partial \Theta} \frac{\partial \Theta}{\partial p_x} = k_B T \frac{\partial f_0}{\partial E} \frac{\partial \Theta}{\partial p_x} \]
\[ \frac{\partial \Theta}{\partial p_x} = \frac{\nu_x}{(k_B T)} \]

(xi)

so (x) becomes
\[ \frac{\partial f_0}{\partial p_x} = \frac{\partial f_0}{\partial E} \nu_x \]

(xii)

Using (ix) and (xii) in (iv), we write the solution to the BTE as
\[ \delta f = -\tau_m \nu_x \frac{\partial f_0}{\partial x} + \tau_m \left[ \frac{d E_C(x)}{dx} - E(k, x) \left( \frac{1}{m^*} \frac{dm^*}{dx} \right) \right] \frac{\partial f_0}{\partial p_x} \]
\[ \text{(xiii)} \]

After simplifying the algebra, the final result:
\[ \delta f = -\tau_m \left( -\frac{\partial f_0}{\partial E} \right) \nu_x \left[ -\frac{d F_n}{dx} + T \left[ E_C(x) + E(k, x) - F_n(x) \right] \frac{d}{dx} \left( \frac{1}{T} \right) \right] \]

is exactly the same as the result for a position-independent bandstructure.

Accordingly, the current equation for a semiconductor with a position-dependent bandstructure is identical to that of a uniform semiconductor:
\[ J_{nn} = \sigma \frac{d (F_n/q)}{dx} - \sigma S \frac{dT}{dx} \]
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

$$J_Q = \frac{1}{\Omega} \sum_k \left( E - F_n \right) \nu_i \delta f$$  \hspace{1cm} (i)

Note that $E$ is the total energy,

$$E = E_c(\bar{r}) + E(\bar{k})$$  \hspace{1cm} (ii)

The solution to the BTE is:

$$\delta f = \tau_m \left( -\frac{\partial f_0}{\partial E} \right) \nu_j \mathcal{F}_j$$  \hspace{1cm} (iii)

where the generalized force is:

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

$$= -\partial_j F_n - \left[ E - F_n(\bar{r}) \right] \frac{1}{T} \partial_j T$$  \hspace{1cm} (iv)

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

$$J_Q = \frac{1}{\Omega} \sum_k \tau_m \left( -\frac{\partial f_0}{\partial E} \right) \nu_i \nu_j \left( E - F_n \right) \left\{ -\partial_j F_n - \left[ E - F_n(\bar{r}) \right] \frac{1}{T} \partial_j T \right\} \right\}$$  \hspace{1cm} (v)

The second term in curly brackets gives the thermal conductivity.

$$\kappa_0 = \frac{1}{\Omega} \sum_k \tau_m \nu_i \nu_j \left( E - F_n \right)^2 \left( -\frac{\partial f_0}{\partial E} \right) \right\}$$