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SOLUTIONS: ECE 656 Exam 5: Fall 2013

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This is a closed book exam. You may use a calculator and the formula sheet at the end of this exam.

There are three equally weighted questions. To receive full credit, you must **show your work** (scratch paper is attached).

The exam is designed to be taken in 50 minutes.

Be sure to fill in your name and Purdue student ID at the top of the page.

DO NOT open the exam until told to do so, and stop working immediately when time is called.

The last page is an equation sheet, which you may remove, if you want.

30 points possible, 10 per question

1) 2 points per part – 10 points total

2a) 5 points
2b) 5 points

3a) 5 points
3b) 5 points

Answer the **five multiple choice questions** below by choosing the **one, best answer**.

1.1) What does "self-scattering" in a Monte Carlo simulation do?

a) Makes the mean-free-path constant.
b) Makes the scattering elastic.
c) Makes the scattering isotropic.
d) Makes the scattering rate constant.
e) Makes the relaxation time approximation apply.

1.2) What is the term, $[\Sigma_1]$, in an NEGF simulation?

a) The Hamiltonian.
b) The broadening for contact one.
c) The self-energy for scattering.
d) The self-energy for contact one.
e) The retarded Green's function.

1.3) When we write a balance equation for the kinetic energy density, *W*, a new unknown is introduced. What is this unknown?

a) The kinetic energy flux.
b) The flux of the kinetic energy flux.
c) The carrier density.
d) The carrier flux.
e) The momentum flux.

1.4) In 3D, we write the current equation as $J_{nj} = nq\mu_n \mathcal{E}_j + (2/3)\mu_n \, dW/dx_j$. How should we write it in 1D?

a) $J_{nj} = nq\mu_n \mathcal{E}_j + (1/3)\mu_n \, dW/dx_j$.
b) $J_{nj} = nq\mu_n \mathcal{E}_j + (1/2)\mu_n \, dW/dx_j$.
c) $J_{nj} = nq\mu_n \mathcal{E}_j + (1)\mu_n \, dW/dx_j$.
d) $J_{nj} = nq\mu_n \mathcal{E}_j + (3/2)\mu_n \, dW/dx_j$
e) $J_{nj} = nq\mu_n \mathcal{E}_j + (2)\mu_n \, dW/dx_j$

1.5) In this lecture, we wrote the general balance equation for a quantity, n_ϕ, as

$\frac{\partial n_\phi}{\partial t} = -\nabla \bullet \vec{F}_\phi + G_\phi - R_\phi$. What assumption is this equation based upon?

a) That the semiconductor is non-degenerate.
b) That the bandstructure is parabolic.
c) That the temperature is uniform.
d) That the electron temperature is equal to the phonon temperature.
e) Only that the BTE is valid.

2) This problem concerns the balance equation for the near-equilibrium heat flux in 3D. For this problem, $\phi(\vec{p}) = (E - E_F)\upsilon_x$ where E is the total energy, $E = E_C + E(\vec{p}) = E_C + \hbar^2 k^2 / (2m^*)$. Note that parabolic bands are assumed.

2a) Evaluate the generation term assuming an *x*-directed electric field. **Do not** assume near-equilibrium conditions.

Solution:

$$G_\phi = -q\mathcal{E}_x \left\{ \frac{1}{\Omega} \sum_{\vec{p}} \frac{\partial \phi}{\partial p_x} f \right\} = -q\mathcal{E}_x \left\{ \frac{1}{\Omega} \sum_{\vec{p}} \frac{\partial \left[(E - E_F)\upsilon_x \right]}{\partial p_x} f \right\}$$

$$G_\phi = -q\mathcal{E}_x \left\{ \frac{1}{\Omega} \sum_{\vec{p}} \left(\frac{\partial E}{\partial p_x} \upsilon_x + (E - E_F) \frac{\partial \upsilon_x}{\partial p_x} \right) f \right\}$$

$$G_\phi = -q\mathcal{E}_x \left\{ \frac{1}{\Omega} \sum_{\vec{p}} \left(\upsilon_x^2 + (E - E_F) \frac{1}{m^*} \right) f \right\}$$

$$G_\phi = -q\mathcal{E}_x \left\{ \frac{1}{\Omega} \sum_{\vec{p}} \left(\upsilon_x^2 + \left(E_C + \frac{1}{2} m^* \upsilon^2 - E_F \right) \frac{1}{m^*} \right) f \right\}$$

$$G_\phi = -q\mathcal{E}_x \left\{ \frac{1}{\Omega} \sum_{\vec{p}} \left(\upsilon_x^2 + \frac{1}{2} \upsilon^2 + \frac{(E_C - E_F)}{m^*} \right) f \right\}$$

The above is an acceptable final answer, but we can express this in terms of averages.

$$G_\phi = -q\mathcal{E}_x \left\{ n\langle \upsilon_x^2 \rangle + \frac{n}{2} \langle \upsilon^2 \rangle + n \frac{(E_C - E_F)}{m^*} \right\}$$

$$G_\phi = -q\mathcal{E}_x \frac{n}{m^*} \left\{ 2\left\langle \frac{1}{2} m^* \upsilon_x^2 \right\rangle + \left\langle \frac{1}{2} m^* \upsilon^2 \right\rangle + (E_C - E_F) \right\}$$

$$\boxed{G_\phi = -\frac{nq}{m^*} \mathcal{E}_x \left\{ 2\left\langle \frac{1}{2} m^* \upsilon_x^2 \right\rangle + \left\langle \frac{1}{2} m^* \upsilon^2 \right\rangle + (E_C - E_F) \right\}}$$

2b) Simplify the result of problem 2a) by assuming near-equilibrium, non-degenerate conditions.

Solution:

Near-equilibrium we can express things in terms of temperature:

$$\left\langle \frac{1}{2} m^* \upsilon^2 \right\rangle = \frac{3}{2} k_B T_L$$

$$\left\langle \frac{1}{2} m^* \upsilon_x^2 \right\rangle = \frac{1}{2} k_B T_L$$

So from problem 2a)

$$G_\phi = -\frac{nq}{m^*} \mathcal{E}_x \left\{ k_B T_L + \frac{3}{2} k_B T_L + \left(E_C - E_F \right) \right\}$$

$$G_\phi = -\frac{nq}{m^*} \mathcal{E}_x k_B T_L \left\{ \frac{5}{2} - \frac{\left(E_F - E_C \right)}{k_B T_L} \right\}$$

$$\boxed{G_\phi = -\frac{nq}{m^*} \mathcal{E}_x k_B T_L \left\{ \frac{5}{2} - \eta_F \right\}}$$

3) This problem concerns the balance equation for the near-equilibrium heat flux in 3D. As in problem 2), $\phi(\vec{p}) = (E - E_F)\upsilon_x$ where E is the total energy, $E = E_C + E(\vec{p}) = E_C + \hbar^2 k^2 / (2m^*)$.

3a) Derive the steady-state, near-equilibrium heat flux, assuming no spatial gradients in the balance equation. You should use the results of problem 2b).

Solution:
The general balance equation:

$$\frac{\partial n_\phi}{\partial t} = -\nabla \bullet \vec{F}_\phi + G_\phi - R_\phi$$

Steady-state, spatially uniform: $R_\phi = G_\phi$, so the balance equation becomes

$$\frac{J_q - J_q^0}{\tau_{Jq}} = \frac{J_q}{\tau_{Jq}} = G_\phi \rightarrow J_q = G_\phi \tau_{Jq}$$

From prob. 2b), we find

$$\boxed{J_q = -\tau_{Jq}\frac{nq}{m^*}\mathcal{E}_x k_B T_L \left\{\frac{5}{2} - \eta_F\right\}}$$

3b) Using the results of problem, 3a), derive an expression for the Peltier coefficient.

Solution:
Need to relate heat current to electrical current: $J_q = \pi J_n$

From 3a)

$$J_q = -\tau_{Jq}\frac{nq}{m^*}\mathcal{E}_x k_B T_L \left\{\frac{5}{2} - \eta_F\right\} = -\frac{\tau_{Jq}}{\tau_m}\left\{nq\left(\frac{q\tau_m}{m^*}\right)\right\}\mathcal{E}_x \frac{k_B T_L}{q}\left\{\frac{5}{2} - \eta_F\right\}$$

$$J_q = -\frac{\tau_{Jq}}{\tau_m}\sigma_n \mathcal{E}_x \frac{k_B T_L}{q}\left\{\frac{5}{2} - \eta_F\right\} = T_L\left(\frac{k_B}{-q}\right)\left\{\frac{5}{2} - \eta_F\right\}\left(\frac{\tau_{Jq}}{\tau_m}\right)J_n$$

Apparently

$$\boxed{\pi = T_L\left(\frac{k_B}{-q}\right)\left\{\frac{5}{2} - \eta_F\right\}\left(\frac{\tau_{Jq}}{\tau_m}\right)}$$

This looks almost like T_L times the expression for the Seebeck coefficient, except for the ratio of scattering times.