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ECE 656 Exam 2: Fall 2017

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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. **Only the Texas Instruments TI-30X IIS scientific calculator is allowed.**

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

The exam is designed to be taken in 75 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 two pages, which list equations may be removed, if you wish.

100 points possible, 25 per question

1) 25 points

2a) 10 points

3a) 5 points

4a) 5 points

2b) 10 points

3b) 10 points

4b) 10 points

2c) 5 points

3c) 5 points

4c) 10 points

3d) 5 points

----- Course policy -----

I understand that if I am caught cheating in this exam, I will earn an F for the course and be reported to the Dean of Students.

Read and understood:

signature

- 1) The mean-free-path for backscattering, λ_0 , is key quantity in the Landauer Approach. Assume n-type Ge doped at $N_D = 10^{15} \text{ cm}^{-3}$. At $T = 300 \text{ K}$, the mobility is:

$$\mu_n = 3200 \text{ cm}^2/\text{V-s}$$

Compute the MFP for backscattering, λ_0 , at $T = 300 \text{ K}$. You may assume that the MFP is independent of energy.

You can make reasonable simplifying assumptions. You will need an effective mass for this calculation. Use the **conductivity effective mass** of n-Ge: $m^* = 0.12m_0$.

HINT: Begin by determining the diffusion coefficient.

- 2) Consider a metallic carbon nanotube, a 1D conductor with a linear dispersion, $E(k_x) = \pm \hbar v_F k_x$. The density of states in this case is a constant, independent of energy, $D(E) = 2g_v / (\pi \hbar v_F)$, where $g_v = 2$ is the valley degeneracy for a carbon nanotube, and v_F is the velocity.
- 2a) Determine the number of channels vs. energy, $M(E)$.
- 2b) If we put a voltage, V , across a nanotube of length, L , a current $I = GV$ will flow. Write down (**but do not evaluate**) an expression for the conductance, G . Your answer should be an integral over energy of a quantity that is fully specified. You should assume linear diffusive transport and a MFP for backscattering that is independent of energy.
- 2c) Assume that the Fermi level is in the conduction band ($E > 0$) and evaluate the integral in 2b) to obtain an expression for conductance in terms of the reduced Fermi level, $\eta_F = (E_F - E_C) / k_B T$, where $E_C = 0$.

3) The Boltzmann Transport Equation is

$$\frac{\partial f}{\partial t} + \vec{v} \cdot \nabla_r f + (-q\vec{E} - q\vec{v} \times \vec{B}) \cdot \nabla_p f = \left. \frac{df}{dt} \right|_{coll}$$

Answer the following questions.

3a) Simplify the BTE for 1D steady-state, no spatial variations, and no B-fields. Assume the Relaxation Time Approximation.

3b) Solve the BTE for a metallic carbon nanotube. That is, find $\delta f(k_x) = f(k_x) - f_0(k_x)$. (Your final answer should include a factor, $(-\partial f_0 / \partial E)$).

3c) From your solution to the BTE in 3c), write down an expression for the current in the nanotube. Your final answer should be in terms of an integral in k-space.

3d) Evaluate the expression in 3c) to find the current in the nanotube. **Assume an energy-independent scattering time.**

- 4) In thermoelectrics, the average energy at which current flows, $E_j = E_C + \Delta_n$ is important. We found that $\Delta_n = 2k_B T$ for a non-degenerate, 3D semiconductor with parabolic energy bands and acoustic deformation potential (ADP) scattering. What is it for a 2D semiconductor with parabolic energy bands and acoustic deformation potential scattering? Answer the following questions.

- 4a) Assume power law scattering:

$$\lambda(E) = \lambda_0 \left[(E - E_C) / (k_B T) \right]^r$$

What is the characteristic exponent, r , for ADP scattering in a 2D, parabolic band semiconductor?

- 4b) The definition of Δ_n is:

$$\Delta_n = \frac{\int (E - E_C) \sigma'_n(E) dE}{\int \sigma'_n(E) dE}$$

Specify the differential conductivity for this problem (i.e. give an equation for it). You may assume a valley degeneracy of two.

4c) Evaluate the integral in 4b) to determine Δ_n in the non-degenerate limit.

SCRATCH PAPER

ECE-656 Key Equations (Weeks 1-9)

Physical constants:

$$\begin{aligned} \hbar &= 1.055 \times 10^{-34} \text{ [J-s]} & m_0 &= 9.109 \times 10^{-31} \text{ [kg]} \\ k_B &= 1.380 \times 10^{-23} \text{ [J/K]} & q &= 1.602 \times 10^{-19} \text{ [C]} & \epsilon_0 &= 8.854 \times 10^{-14} \text{ [F/cm]} \end{aligned}$$

Density of states in k-space:

$$\begin{aligned} \text{1D: } N_k &= 2 \times (L/2\pi) = L/\pi & \text{2D: } N_k &= 2 \times (A/4\pi^2) = A/2\pi^2 & \text{3D:} \\ N_k &= 2 \times (\Omega/8\pi^2) = \Omega/4\pi^3 \end{aligned}$$

Density of states in energy (parabolic bands, per length, area, or volume):

$$D_{1D}(E) = \frac{g_v}{\pi \hbar} \sqrt{\frac{2m^*}{E - \epsilon_1}} \quad D_{2D}(E) = g_v \frac{m^*}{\pi \hbar^2} \quad D_{3D}(E) = g_v \frac{m^* \sqrt{2m^*(E - E_C)}}{\pi^2 \hbar^3}$$

Fermi function and Fermi-Dirac Integrals / Bose-Einstein function

$$\begin{aligned} f_0(E) &= \frac{1}{1 + e^{(E - E_F)/k_B T}} & N_0 &= \frac{1}{e^{h\omega_0/k_B T} - 1} \\ \mathcal{F}_j(\eta_F) &= \frac{1}{\Gamma(j+1)} \int_0^\infty \frac{\eta^j d\eta}{1 + e^{\eta - \eta_F}} & \mathcal{F}_j(\eta_F) &\rightarrow e^{\eta_F} \quad \eta_F \ll 0 & \frac{d\mathcal{F}_j}{d\eta_F} &= \mathcal{F}_{j-1} \\ \Gamma(n) &= (n-1)! \quad (n \text{ an integer}) & \Gamma(1/2) &= \sqrt{\pi} & \Gamma(p+1) &= p\Gamma(p) \end{aligned}$$

Scattering:

$$\begin{aligned} S(\vec{p}, \vec{p}') &= \frac{2\pi}{\hbar} |H_{\vec{p}', \vec{p}}|^2 \delta(E' - E - \Delta E) & H_{\vec{p}', \vec{p}} &= \frac{1}{\Omega} \int_{-\infty}^{+\infty} e^{-i\vec{p}' \cdot \vec{r}/\hbar} U_S(\vec{r}) e^{i\vec{p} \cdot \vec{r}/\hbar} d\vec{r} \\ \frac{1}{\tau(\vec{p})} &= \sum_{\vec{p}', \uparrow} S(\vec{p}, \vec{p}') & \frac{1}{\tau_m(\vec{p})} &= \sum_{\vec{p}', \uparrow} S(\vec{p}, \vec{p}') \frac{\Delta p_z}{p_{z0}} & \frac{1}{\tau_E(\vec{p})} &= \sum_{\vec{p}', \uparrow} S(\vec{p}, \vec{p}') \frac{\Delta E}{E_0} \\ \text{ADP: } |K_q|^2 &= q^2 D_A^2 & \text{ODP: } |K_q|^2 &= D_0^2 & \text{PZ: } |K_q|^2 &= (e e_{PZ} / \kappa_S \epsilon_0)^2 & \text{POP: } |K_\beta|^2 &= \frac{\rho e^2 \omega_0^2}{q^2 \kappa_0 \epsilon_0} \left(\frac{\kappa_0}{\kappa_\infty} - 1 \right) \\ S(\vec{p}, \vec{p}') &= \frac{\pi}{\Omega \rho \omega} |K_q|^2 \left(N_\omega + \frac{1}{2} \mp \frac{1}{2} \right) \delta(\vec{p}' - \vec{p} \mp \hbar \vec{q}) \delta(E' - E \mp \hbar \omega) \\ \delta(\vec{p}' - \vec{p} \mp \hbar \vec{q}) \delta(E' - E \mp \hbar \omega) &\rightarrow \frac{1}{\hbar v q} \delta \left(\pm \cos \theta + \frac{\hbar q}{2p} \mp \frac{\omega_q}{v q} \right) \\ \frac{1}{\tau} &= \frac{1}{\tau_{abs}} + \frac{1}{\tau_{ems}} = \frac{2\pi}{\hbar} \left(\frac{D_A^2 k_B T}{c_i} \right) \frac{D_{3D}(E)}{2} \quad (\text{ADP}) & L_D &= \sqrt{\frac{\kappa_S \epsilon_0 k_B T}{q^2 n_0}} \\ \frac{1}{\tau} &= \frac{1}{\tau_m} = \frac{2\pi}{\hbar} \left(\frac{\hbar D_0^2}{2\rho \omega_0} \right) \left(N_0 + \frac{1}{2} \mp \frac{1}{2} \right) \frac{D_{3D}(E \pm \hbar \omega_0)}{2} & N_0 &= \frac{1}{e^{h\omega_0/k_B T} - 1} \quad (\text{ODP}) \end{aligned}$$

Boltzmann Transport Equation:

$$\frac{\partial f}{\partial t} + \vec{v} \cdot \nabla_r f + \vec{F}_e \cdot \nabla_p f = \frac{df}{dt} \Big|_{coll} \quad \vec{F}_e = -q\vec{E} - q\vec{v} \times \vec{B} \quad \frac{df}{dt} \Big|_{coll} = -\frac{(f - f_s)}{\tau_m} = -\frac{\delta f}{\tau_m} \quad (\text{RTA})$$

With a small B-field, the resulting 2D current equation is $\vec{J}_n = \sigma_s \vec{E} - \sigma_s \mu_H (\vec{E} \times \vec{B})$

$$(\omega_c \tau_m \ll 1)$$

$$\mu_H = \mu_n r_H \quad r_H \equiv \frac{\langle \tau_m^2 \rangle}{\langle \tau_m \rangle^2} \quad \langle \langle \bullet \rangle \rangle \equiv \langle (\bullet) E \rangle / \langle E \rangle$$

Isothermal Near-Equilibrium Transport: Summary of Landauer Approach

$$I = \frac{2q}{h} \int \mathcal{T}(E) M(E) (f_1 - f_2) dE \rightarrow \text{small bias, isothermal: } f_1(E) - f_2(E) = \left(-\frac{\partial f_0}{\partial E} \right) (qV)$$

Linear response (also called low bias, near-equilibrium):

$$I = GV \quad G = \frac{2q^2}{h} \int \mathcal{T}(E) M(E) \left(-\frac{\partial f_0}{\partial E} \right) dE \quad G = \frac{2q^2}{h} \langle \langle \mathcal{T}(E) \rangle \rangle \langle \langle M(E) \rangle \rangle$$

$$\langle \langle \mathcal{T}(E) \rangle \rangle \equiv \left\{ \frac{\int \mathcal{T}(E) M(E) (-\partial f_0 / \partial E) dE}{\int M(E) (-\partial f_0 / \partial E) dE} \right\} \quad \langle \langle M(E) \rangle \rangle = \int M(E) (-\partial f_0 / \partial E) dE$$

$$R_{ball} = \frac{1}{M(E_F)} \frac{h}{2q^2} = \frac{12.8 \text{ k}\Omega}{M}$$

Modes / channels (general):

$$M(E) \equiv \frac{h}{4} \langle \mathbf{v}_x^+(E) \rangle D_{1D}(E) \quad \langle \mathbf{v}_x^+(E) \rangle = v(E)$$

$$M(E) = WM_{2D} \equiv W \frac{h}{4} \langle \mathbf{v}_x^+(E) \rangle D_{2D}(E) \quad \langle \mathbf{v}_x^+(E) \rangle = \frac{2}{\pi} v(E)$$

$$M(E) = AM_{3D} \equiv A \frac{h}{4} \langle \mathbf{v}_x^+(E) \rangle D_{3D}(E) \quad \langle \mathbf{v}_x^+(E) \rangle = \frac{1}{2} v(E)$$

Modes (Parabolic bands): $(E(k) = E_C + \hbar^2 k^2 / 2m^*)$

$$M(E) = M_{1D}(E) = g_v$$

$$M(E) = WM_{2D}(E) = g_v W \frac{\sqrt{2m^*(E - E_C)}}{\pi \hbar}$$

$$M(E) = AM_{3D}(E) = g_v A \frac{m^*}{2\pi \hbar^2} (E - E_C)$$

Modes (graphene):

$$M(E) = W 2|E| / \pi \hbar v_F$$

Transmission: $\mathcal{T}(E) = \frac{\lambda(E)}{\lambda(E) + L}$

Mean-free-path for backscattering:

$$1D: \lambda(E) = 2v(E)\tau_m(E) \quad 2D: \lambda(E) = \frac{\pi}{2}v(E)\tau_m(E) \quad 3D: \lambda(E) = \frac{4}{3}v(E)\tau_m(E)$$

Diffusion coefficient: $D_n = \langle v_x^+ \rangle \langle \lambda \rangle / 2$ $D_n = v_T \lambda_0 / 2$ $D_n(E) = \langle v_x^+(E) \rangle \lambda(E) / 2$

Uni-directional thermal velocity: $\langle v_x^+ \rangle = v_T = \sqrt{2k_B T / \pi m^*}$ ($\eta_F \ll 0$)

Thermoelectric transport:

Coupled current equations (diffusive): $J_x = \sigma E_x - \sigma S dT/dx$ $J_x^Q = T \sigma S E_x - \kappa_0 dT/dx$

Coupled current equations (inverted): $E_x = \rho J_x + S \frac{dT_L}{dx}$ $J_x^Q = \pi J_x - \kappa_e \frac{dT}{dx}$

Transport coefficients:

$$\sigma = \int \sigma'(E) dE = \frac{2q^2}{h} \langle M \rangle \langle \lambda \rangle \quad \sigma'(E) = \frac{2q^2}{h} \lambda(E) \frac{M(E)}{A} \left(-\frac{\partial f_0}{\partial E} \right) \quad \langle M \rangle = \int M(E) \left(-\frac{\partial f_0}{\partial E} \right) dE$$

$$S = -\frac{k_B}{q} \int \left(\frac{E - E_F}{k_B T} \right) \sigma'(E) dE \bigg/ \int \sigma'(E) dE = -\left(\frac{k_B}{q} \right) \left\langle \frac{E - E_F}{k_B T} \right\rangle = \left(\frac{k_B}{-q} \right) \left\{ \frac{(E_C - E_F)}{k_B T} + \frac{\Delta_n}{k_B T} \right\}$$

$\pi = T_L S$ (Kelvin Relation)

$$\kappa_0 = T \left(\frac{k_B}{q} \right)^2 \int \left(\frac{E - E_F}{k_B T} \right)^2 \sigma'(E) dE = \kappa_0 = \sigma T \left(\frac{k_B}{q} \right)^2 \left\{ \left(\frac{E - E_F}{k_B T} \right)^2 \right\}_{\text{ave}} \quad \kappa_e = \kappa_0 - \pi S \sigma$$

$$\frac{\kappa_e}{\sigma} = \left(\frac{k_B}{q} \right)^2 \left\{ \left\langle \left(\frac{E - E_F}{k_B T} \right)^2 \right\rangle - \left\langle \left(\frac{E - E_F}{k_B T} \right) \right\rangle^2 \right\} T = LT \quad \text{(Weidemann-Franz "Law")}$$

$$2 \left(\frac{k_B}{q} \right)^2 < L < \frac{\pi^2}{3} \left(\frac{k_B}{q} \right)^2 \quad (\text{parabolic bands with energy-independent scattering})$$

Thermoelectric material Figure of Merit: $zT = \frac{S^2 \sigma T}{\kappa}$

Lattice thermal conductivity: $\kappa_L = \frac{\pi^2 k_B^2 T_L}{3h} \int \lambda_{ph}(\hbar\omega) \frac{M_{ph}(\hbar\omega)}{A} W_{ph}(\hbar\omega) d(\hbar\omega)$