HW#6 Solutions, Chapter 11, Problems 1-3

Problem 1: Electron-ionized-impurity scattering via the screened Coulomb potential

(a) According to the hydrogenic corollary to the effective mass theorem, an ionized impurity embedded in a crystal of permittivity ε_r can be modeled as a Coulomb potential. If the crystal is a conductor having significant free carrier concentration, that Coulomb potential must be screened:

$$V(r) = \frac{\pm q_S}{4\pi\varepsilon_r\varepsilon_0 r}\exp(-r/L_D) \tag{1}$$

where q_S is the charge of the ionized impurity, L_D is the Debye screening length at low carrier concentrations (or high temperatures) and is the Thomas-Fermi screening length at high concentrations (or low temperatures). Multiplication of (1) bv the particle charge q_p creates a potential energy which acts like a perturbation to Bloch electrons. Defining k_1 and k_2 as the incident and final Bloch wave vectors, we can then treat (1) as a perturbation Hamiltonian in quantum mechanics with an expectation value given by

$$H_{k_2,k_1} \equiv <\psi_{k_2}|H'|\psi_{k_1}> = <\psi_{k_2}|qV(r)|\psi_{k_1}> = \frac{q_P q_S}{4\pi\varepsilon_r\varepsilon_0 V}\int \frac{\exp(-r/L_{D)}}{r}\exp\left[\, j\left(\vec{k}_1 - \vec{k}_2\right)\cdot\vec{r}\,\right] d^3r \tag{2}$$

where < | denotes a "bra" state in Hilbert space, and | > denotes a "ket" state. Only the envelope portion of the Bloch functions have been retained in (2), the cell-periodic portion assumed to be maintained in the scattering processes and, therefore, normalized out of the integral. By choosing spherical coordinates for (2) in k space, we can write

$$H_{k_2,k_1} = \frac{q_P q_S}{4\pi\varepsilon_r\varepsilon_0 V}\int\int\int \frac{\exp(-r/L_{D)}}{r}\exp\left[\, j\left(\vec{k}_1 - \vec{k}_2\right)\cdot\vec{r}\,\right] r^2\sin\theta\, dr\, d\theta\, d\phi \tag{3}$$

This canbe solved simply by first defining the direction of the vector $\vec{k}_1 - \vec{k}_2$ (which is fixed during the integration) arbitrarily along the z axis of a same spherical coordinate system. Hence, $\left(\vec{k}_1 - \vec{k}_2\right)\square\vec{r} = |\vec{k}_1 - \vec{k}_2||\vec{r}|\cos\theta \equiv \Delta k\cdot r\cdot\cos\theta$, and there is no dependence on azimuthal angle, so that (3) becomes,

$$H_{k_2,k_1} = \frac{q_P q_S}{2\varepsilon_r\varepsilon_0 V}\int\int \frac{\exp(-r/L_{D)}}{r}\exp\left[\, j\left(\Delta k\cdot r\right)\cos\theta\,\right] r^2\sin\theta\, dr\, d\theta \tag{4}$$

The θ integral is straightforward and yields

$$H_{k_2,k_1} = \frac{q_P q_S}{2\varepsilon_r \varepsilon_0 V}\int \frac{\exp(-r/L_{D)}}{r} r^2 dr \cdot \left(\frac{-\exp\left[\, j\left(\Delta k \cdot r\right)\cos\theta \,\right]}{j(\Delta k \cdot r)} \Bigg|_0^{\pi} \right)$$

$$= \frac{q_P q_S}{\varepsilon_r \varepsilon_0 V}\int_0^{\infty} \exp(-r/L_D)\frac{\sin(\Delta k \cdot r)}{\Delta k} dr$$

From standard integral tables or a good symbolic integration tool, this can be evaluated as

$$= \frac{q_P q_S}{\varepsilon_r \varepsilon_0 V \Delta k}\left\{ \exp(-r/L_D)\frac{[(-1/L_D)\sin \Delta k r - \Delta k \cos(\Delta k r)]}{[(1/L_D)^2 + (\Delta k)^2]} \right\}\Bigg|_0^{\infty}$$

$$H_{k_2,k_1} = \frac{q_P q_S}{\varepsilon_r \varepsilon_0 V[(1/L_D)^2 + (\Delta k)^2]} \quad , \tag{5}$$

a remarkably simple result. To turn this into a differential scattering cross section for use in transport calculations, we note from the trigonometry in the figure to the right that $\Delta k = 2k_1 \sin(\theta/2)$ Hence, from the central result of the quantum mechanical scattering theory,

$$\sigma(\theta) \approx \frac{V^2 (m^*)^2}{(2\pi)^2 \hbar^4} |H_{\vec{k}_2,\vec{k}_1}(k_1 = k_2)|^2 = \frac{(m^*)^2}{(2\pi\varepsilon_r\varepsilon_0)^2 \hbar^4}\left(\frac{q_P q_S}{(1/L_D)^2 + 4k_1^2 \sin^2\theta/2} \right)^2 \tag{6}$$

$$= \frac{(m^*)^2}{(2\pi\varepsilon_r\varepsilon_0)^2 (2\hbar k_1)^4}\left(\frac{q_P q_S}{(\beta)^{-2} + \sin^2\theta/2} \right)^2 = \left[\frac{e^2/(8\pi\varepsilon_r\varepsilon_0 m^* v^2)}{\sin^2(\theta/2) + \beta^{-2}} \cdot \right]^2 \tag{7}$$

where $\beta = 2kL_D$ and the last step uses $m^* v^2 = (\hbar k)^2 / m^*$. One remarkable effect is evident in (7) – the cross section does not depend on the relative signs between incident particle and scatterer !

(b) To turn (7) into a momentum relaxation time, we start with a trigonometric identity $\sin^2(\theta/2) = (1/2)(1-\cos\theta)$, and then substitute into the transport integral

$$1/\tau_m = 2\pi n_I v \cdot \int_0^{\pi} \sigma(\theta)(1-\cos\theta)\sin\theta d\theta \tag{8}$$

where n_I is the concentration of ionized impurities. The first term in the integrand on the RHS of (8), that goes as $\sin\theta$, is an odd function with respect to the center of the integration domain, $\theta = \pi/2$, whereas the θ-dependence of (8) is even. So the first term of (8) vanishes. The second term, through a good integral table or symbolic match tool yields,

$$1/\tau_m = \frac{nm*}{(8\pi)\hbar^3 k_1^3}\left(\frac{q_P q_S}{\varepsilon_r \varepsilon_0}\right)^2 [\ln(1+\beta^2) - \beta^2/(1+\beta^2)] \tag{9}$$

where $\beta \equiv 2k_1 L_D$. Using the spherical-band relation $(\hbar k_1^2)/(2m^*) = U_1$, we get

$$\tau_m = \frac{(2m*)^{1/2}(16\pi)U_1^{3/2}}{n_I}\left(\frac{\varepsilon_r \varepsilon_0}{q_P q_S}\right)^2 [\ln(1+\beta^2) - \beta^2/(1+\beta^2)]^{-1} \tag{10}$$

(c) To do transport evaluation, (10) should be averaged over the Maxwell-Boltzmann particle distribution function to get $<\tau_m>$. But the expression in square brackets clearly depends on energy through the definition of β. Fortunatelyu, its dependence is much weaker than the dominant term $(U_1)^{3/2}$ since in the spherical-valley approximation $U = (\hbar k)^2/2m*$ or $k = \sqrt{2mU}/\hbar$. So we treat this expression as a constant C during the integration

$$\ln[(1+\beta^2) - \beta^2/(1+\beta^2)] \equiv C \quad , \quad \tau(U) \approx \frac{16\pi\sqrt{2m}}{CN_I}\left[\frac{\varepsilon_r \varepsilon_0}{q_p q_s}\right]^2 U^{3/2}$$

This allows us to integrate (10) using our previous result for the generic form $\tau(U) = AU^{-S}$ averaged over the MB distribution: $< \tau_m >= \frac{4A \cdot \Gamma(5/2 - S)}{3\sqrt{\pi}(k_B T)^S}$ where $A = \frac{16\pi\sqrt{2m^*}}{CN_I}\left(\frac{\varepsilon_r \varepsilon_0}{q_p q_s}\right)^2$

Since S = -3/2, Γ(5/2-S) = Γ(4) = 3! = 6, finally get

$$< \tau_m >= \frac{128\sqrt{2\pi m*}}{CN_I}\left(\frac{\varepsilon_r \varepsilon_0}{q_p q_s}\right)^2 (k_B T)^{3/2} \tag{11}$$

Problem 2: Electron-acoustic-phonon scattering via the deformation potential

(a) The Bardeen-Shockley proof utilizes elasticity theory to relate the band-edge energy to the *strain* η through the relation:

$$\delta U_P = \Xi\, \eta \tag{1}$$

where Ξ is the deformation-potential constant - generally a known parameter for most semiconductors having a value between ~5 and 10 eV. Associated with any time-varying strain are lattice waves of the form:

$$\vec{u} = A\exp[\pm j(\vec{k}_p \cdot \vec{r})]\hat{k}_p \tag{2}$$

where u is the *deformation* at each lattice away from the equilibrium position, A is the amplitude, k_p is the phonon wave vector, and ω_p is the circular frequency associated with the dispersion curve ω vs kp. From the fundamental definition of strain in elasticity theory,

$$\eta \equiv \vec{\nabla} \cdot \vec{u} = \pm j(\vec{k}_p \cdot \vec{u}) \tag{3}$$

For longitudinal modes, u and k_p are parallel so that $\eta = \pm jk_p u$, and (1) becomes

$$\delta U_P = j\,\Xi\, k_p\, u \quad = j\,\Xi\, k_p\, A\exp[j(\mathbf{k_p}\cdot\mathbf{r})] \tag{4}$$

This can be used as a transition Hamiltonian with the understanding that $H_{k1,k2} = \delta U_P$, leading to

$$|H_{k_2,k_1}| = \left| \frac{j\Xi k_p A}{V} \int \exp[\, j(\vec{k}_1 - \vec{k}_2 \pm \vec{k}_p) \cdot \vec{r}\,] d^3 r \right|$$

where V is the sample volume, needed for normalization of the wave functions. Since there are no external forces at work, whatever happens between the electrons and phonons should conserve total crystal-momentum conservation, (assuming of course that the electrons stay within the same band and that no photons are generated). Hence we can write:

$$\vec{k}_1 - \vec{k}_2 \pm \vec{k}_p = 0$$

and

$$|H_{k_2,k_1}| = \left| \frac{j\Xi k_p A}{V} \int d^3 r \right| = \Xi \cdot k_p A \tag{5}$$

This is a form that substitutes directly into Fermi's Golden rule for the quantum-mechanical scattering transition rate. But before doing that, we need some quantum mechanical form for the lattice-wave amplitude. Earlier in the discussion of lattice waves and phonons, we derived (also see Kittel Chap. 4):

$$A^2 = \frac{4(< n_k > +1/2)\hbar}{\omega_p \rho V}$$

where $<n_k>$ is the occupancy for the phonons (Planck function), ω_p is the phonon dispersion relation, ρ is the density, and V is the volume of the sample.

In our acoustical (long-wavelength) approximation and at low enough temperature, we have

$$< n_k >= \frac{1}{\exp(\hbar\omega / k_B T) - 1} \approx \frac{k_B T}{\hbar\omega} >> 1$$

And $\omega \approx (C_{mm}/\rho)^{1/2}\, k$ where C_{mm} is the longitudinal stiffness coefficient (along the same direction as the phonon propagation). Hence, we get

$$|H_{k_2,k_1}| = \Xi \cdot [k_B T / (2VC_{mm})]^{1/2} \tag{6}$$

This is a physically profound expression that combines effects of band structure, statistical mechanics, and elasticity theory all in one elegant expression !

(b) Now we are ready to apply Fermi's golden rule to get the transport parameters. But we need to account for phonon absorption and phonon emission as separate processes, since both are tantamount to scattering of an electron. Since the electron and phonon energies are all internal to the crystal, they both conserve crystal energy. So the overall transition rate for both can be written

$$R_{1,2} = \frac{\pi k_B T}{\hbar V C_{mm}} \Xi^2 \{\delta[U(\vec{k}_2 - \vec{k}_p) - U(\vec{k}_1)] + \delta[U(\vec{k}_2 + \vec{k}_p) - U(\vec{k}_1)]\} \qquad (7)$$

But for acoustical phonons, we expect the phonon-induced energy change for most electrons to be negligible compared to their incident kinetic energy. So we approximate each scattering event as *inelastic* with respect to the electron energy:

$$U(\vec{k}_2 - \vec{k}_p) \approx U(\vec{k}_2 + \vec{k}_p) \approx U(\vec{k}_2)$$

The easiest route to the momentum relaxation time is just the integral

$$\frac{1}{\tau_m} \approx \frac{V}{(2\pi)^2} \int \left(\int R_{1,2} k_2^2 dk_2 \right) (1 - \cos\theta_2) \sin\theta_2 d\theta_2 \qquad (8)$$

Given that (7) does not depend on angle, this becomes

$$\frac{1}{\tau_m} \approx \frac{k_B T}{2\pi\hbar C_{mm}} \Xi^2 \int k_2^2 \left[\delta[U(\vec{k}_2) - U(\vec{k}_1)] + \delta[U(\vec{k}_2) - U(\vec{k}_1)] \right] dk_2$$

where the θ integral was carried out using the fact that the term cosθsinθdθ vanishes over the range from 0 to π. *We must be careful using the Dirac delta function,* and convert from dk_1 to dU_1 taking advantage of the spherical-band approximation that pervades scattering theory:

$$\frac{1}{\tau_m} \approx \frac{k_B T}{2\pi\hbar C_{mm}} \Xi^2 \int k_2^2 \left[\delta[U(\vec{k}_2) - U(\vec{k}_1)] + \delta[U(\vec{k}_2) - U(\vec{k}_1)] \right] \frac{m^*}{\hbar^2 k_2} dU_2$$

$$\frac{1}{\tau_m} \approx \frac{m^* k_B T}{2\pi\hbar^3 C_{mm}} \Xi^2 \int k_2 \left[\delta[U(\vec{k}_2) - U(\vec{k}_1)] + \delta[U(\vec{k}_2) - U(\vec{k}_1)] \right] dU_2$$

$$\frac{1}{\tau_m} \approx \frac{m^* k_B T}{\pi\hbar^3 C_{mm}} \Xi^2 k_1$$

where the last step uses the *sifting property* of the Dirac delta function. Finally using the spherical band approximation one last time, $k_1 = (2m^*U)^{1/2}/\hbar$, we get

$$\frac{1}{\tau_m} \approx \frac{m^* k_B T}{\pi\hbar^3 C_{mm}} \Xi^2 (2m^*U)^{1/2}/\hbar = \frac{(2)^{1/2}(m^*)^{3/2} k_B T}{\pi\hbar^4 C_{mm}} \Xi^2 U^{1/2}$$

or $$\tau_m = \frac{\pi\hbar^4 C_{mm}}{(2)^{1/2}(m^*)^{3/2}k_B T\Xi^2}U^{-1/2} \qquad (9)$$

This expression is sometimes written in an alternative but equivalent form using the fact that the (spin-independent) specific density of free carrier states in a spherical valley is given by

$$g'(U) = \frac{1}{4\pi^2}\left(\frac{2m^*}{\hbar^2}\right)^{3/2}U^{1/2}$$

and the speed of sound for longitudinal acoustic waves is given by $(v_S)^2 = (C_{mm}/\rho)$. Thus,

$$\tau_L(U) = \frac{\hbar\rho v_s^2}{2\pi k_B T g(U)\Xi^2} \qquad (10)$$

(c) The expression (9) can be written in the form $\tau_m \equiv AU^{-S}$ where the last step defines the energy-dependent exponent S = 1/2. This allows us to do the averaging $<\tau_m>$ over the Maxwell-Boltzmann distribution using the formula derived previouisly

$$<\tau_m> = \frac{4A\cdot\Gamma(5/2-S)}{3\sqrt{\pi}\,(k_B T)^S} = \frac{\dfrac{4\pi\hbar^4 C_{mm}}{(2)^{1/2}(m^*)^{3/2}k_B T\cdot\Xi^2}\cdot\Gamma(5/2-1/2)}{3\sqrt{\pi}\,(k_B T)^S} = \frac{(2/3)\sqrt{2\pi}\hbar^4 C_{mm}}{(m^*)^{3/2}\Xi^2(k_B T)^{3/2}}$$

$$<\mu> = \frac{e<\tau_m>}{m^*} = \frac{e(2/3)\sqrt{2\pi}\hbar^4 C_{mm}}{(m^*)^{5/2}\Xi^2(k_B T)^{3/2}} = \frac{e(2/3)\sqrt{2\pi}\hbar^4\rho v_S^2}{(m^*)^{5/2}\Xi^2(k_B T)^{3/2}} \qquad (11)$$

This allows us to calculate the (small-field) mobility of free carriers in a spherical band having. Let's suppose m* == 0.17 m_0, Ξ = 10 eV, ρ = 5.3 gm/cm^3 and v_s = 3000 m/s. Substituting these parameters into (11), we get μ = 0.25 m^2/V-s (2.4x10^3 cm^2/V-s) at 300 K, and get μ = 1.9 m^2/V-s (1.9x10^4 cm^2/V-s).

3. Electron-Phonon Scattering in Different Semiconductors

(a) The *potential energy* of carrier is being perturbed, specifically the electrostatic potential energy.

(b) (i) ε_{mm} is dielectric constant, (ii) C_{mm} = stiffness coefficient, (iii) e_{mm} = piezoelectric stress coefficient, (iv) n_{cell} = density of primitive unit cells, (v) Q_{eff} = effective charge per cell and (vi) $\hbar\omega_0$ = the optical phonon energy.

(c) AlN will be most impacted by (E.1) because it has the greatest piezoelectric stress coefficient ?

(d) Ge will be the least impacted by (E.2) because it is non-polar.

(e) A bit of number crunching yields for GaAs and piezoelectric scattering $<\mu> = 62\ m^2/V\text{-}s = 6.2x10^5\ cm^2/V\text{-}s$. For GaAs and LO phonon scattering $<\mu> = 0.94\ m^2/V\text{-}s = 9.4x10^3\ cm^2/V\text{-}s$.