Scattering Test

```
clc
clear
close all

q = 1.602e-19; % C
E_field = linspace(0, 2, 6) * q; % electric field in J
h = 6.626e-34; % Joule seconds
h_bar = h / (2*pi); % Joule seconds
KB_J = 1.381e-23; % Boltzmann constant in J/K
T = 298; % room temperature at degrees K
N = 1000; % number of particles
m_e = 9.109e-31; % electron rest mass in kg
m_gamma = 0.067 * m_e; % effective mass of electron in gamma valley
m_X_LO = 1.3 * m_e; % longitudinal effective mass of electron in X valley
m_X_TA = 0.23 * m_e; % transverse effective mass of electron in X valley
m_L_LO = 1.9 * m_e; % longitudinal effective mass of electron in L valley
m_L_TA = 0.075 * m_e; % transverse effective mass of electron in L valley
m_eff = [m_gamma (m_X_LO * m_X_TA^2)^(1/3) (m_L_LO * m_L_TA^2)^(1/3)];
E_phonon = 36.25e-3 * q; % energy of a phonon in GaAs in J
w_LO = 5.52e13; % rad/s for phonon in GaAs
e_s = 12.9; % static dielectric constant
e_inf = 10.9; % high-frequency dielectric constant
e_0 = 8.854e-12; % vacuum permittivity in F/m
t_max = 10e-12; % length of simulation (10 picoseconds)
t_ensemble = 1e-12; % length of ensemble (1 picoseconds)
dt = 10e-15; % length of unit of time (10 femtoseconds)
N_0 = 1 / (exp(E_phonon / (KB_J * T)) - 1); % phonon occupation number
p = 5320; % mass density of GaAs, kg/m^3
```

Initial Values

```
rng(6712); % the random number seed I spammed on my keyboard
E_kin = linspace(0, 2, 1000) * q;
phi = 2 * pi * rand(N, 1);
theta = acos(1 - 2 * rand(N, 1));
k = sqrt((2 * m_gamma * E_kin) / (h_bar ^ 2));
k_x = k .* sin(theta) .* cos(phi);
k_y = k .* sin(theta) .* sin(phi);
k_z = k .* cos(theta);
valley_index = ones(N, 1); % gamma is 1, X is 2, L is 3
m_valley = valley_index;
Z_if = [0 3 4
        1 0 4
        1 3 0]; % # of final vallies
D_if = [0 9.5 9
        9.5 0 6.5
        9 6.5 0] * (q / 1e-10); % from eV / Angstrom to J/m
w_if = [0 .048 .035
```

```
        .048 0 .042
        .035 .042 0] * q / h_bar;
E_if = [0 .49 .29
       -.49 0 .2
       -.29 -.2 0] * q;
D0 = [8.5 9.5 11] * q; % Deformation potential in J for gamma, X, L valley
v_s = 5110; % sound velocity in GaAs in m/s
```

Polar-Optical-Phonon Scattering

```
function pop_scatter = scatter_pop(E, m, h_bar, w_0, E_phonon, KB_J, q, e_inf, e_s,
e_0, T)
    pop_scatter = size(E);
    for i = 1:length(E)
        x = h_bar * w_0 / E(i);
        C = ((q^2 * w_0) / (8 * pi * e_0)) * sqrt(2 * m / (h_bar^2)) * ...
            ((1 / e_inf) - (1 / e_s)) * (1 / sqrt(E(i)));
        N_0 = 1 / (exp(E_phonon / (KB_J * T)) - 1);

        if E(i) > (h_bar * w_0)
            pop_scatter(i) = C * (N_0 * log(abs((1 + sqrt(1 + x)) / (-1 + sqrt(1 +
x)))) + ...
                (N_0 + 1) * log(abs((1 + sqrt(1 - x)) / (1 - sqrt(1 - x)))));
        else
            pop_scatter(i) = C * (N_0 * log(abs((1 + sqrt(1 + x)) / (-1 + sqrt(1 +
x)))));
        end
    end
end
```

Acoustic

```
function acoustic = ac_scatter(E, m, h_bar, p, v_s, D, KB_J, T)
    acoustic = (D^2 * KB_J * T) / (2 * pi * h_bar * p * v_s^2) * ...
        ((2 * m) / (h_bar ^ 2)) ^ 1.5 * sqrt(E);
end
```

Intervalley Scattering

```
function gamma_inter_abs = inter_scatter_abs(E, h_bar, KB_J, T, D_if, Z_if, w_if,
E_if, m_final, p)
    gamma_inter_abs = zeros(1, length(E));
    for j = 1:length(E)
        N_if = 1 / (exp(h_bar * w_if / (KB_J * T)) - 1);
        g_DOS = DOS(E(j) + (h_bar * w_if) - E_if, m_final, h_bar);
        gamma_inter_abs(j) = N_if * (pi * D_if^2 * Z_if / (2 * p * w_if)) * g_DOS;
    end
end
```

```
function gamma_inter_emit = inter_scatter_emit(E, h_bar, KB_J, T, D_if, Z_if, w_if,
E_if, m_final, p)
    gamma_inter_emit = zeros(1, length(E));
    for j = 1:length(E)
        N_if = 1 / (exp(h_bar * w_if / (KB_J * T)) - 1);
        g_DOS = DOS(E(j) - (h_bar * w_if) - E_if, m_final, h_bar);
        gamma_inter_emit(j) = (N_if + 1) * (pi * D_if^2 * Z_if / (2 * p * w_if)) *
g_DOS;
    end
end
```

DOS

```
function g_DOS = DOS(E, m, h_bar)
    if E > 0
        g_DOS = (sqrt(E) / (2 * (pi^2))) * (2 * m / (h_bar ^ 2)) ^ 1.5;
    else
        g_DOS = 0;
    end
end
```

Graphing

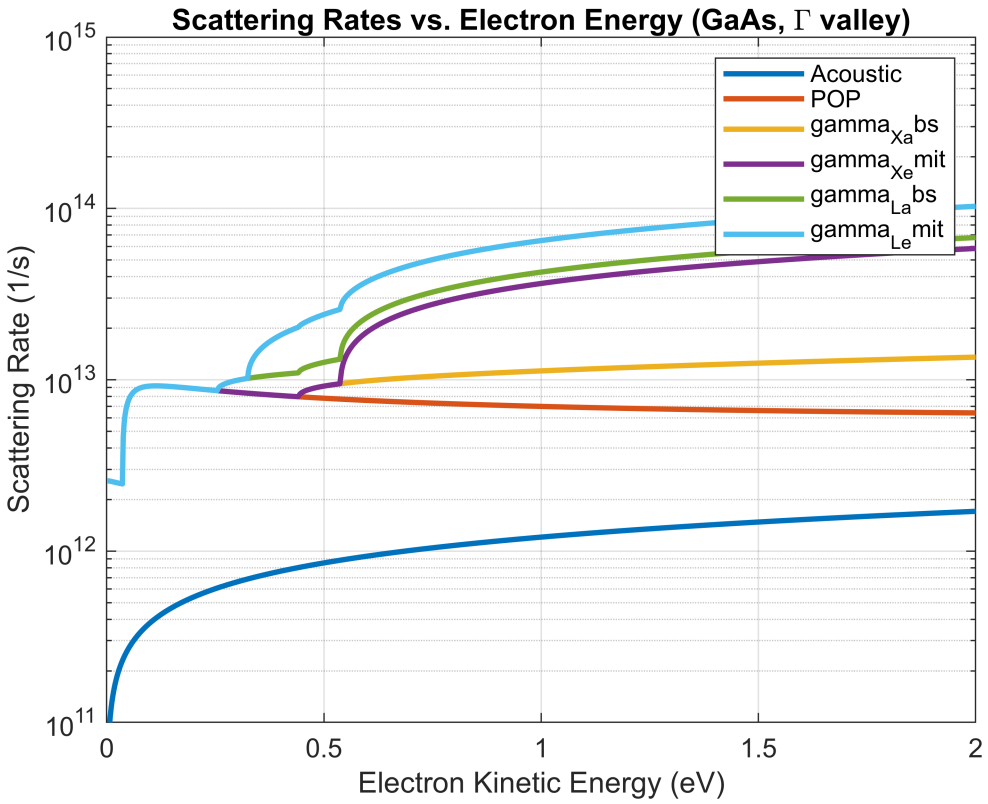
Gamma Scattering

```
x = 1;
gamma_1 = ac_scatter(E_kin, m_eff(x), h_bar, p, v_s, D0(x), KB_J, T);
gamma_2 = scatter_pop(E_kin, m_eff(x), h_bar, w_LO, E_phonon, KB_J, q, e_inf, e_s,
e_0, T) + gamma_1;
% Gamma --> X
y = 2;
gamma_3 = inter_scatter_abs(E_kin, h_bar, KB_J, T, D_if(x, y), Z_if(x, y), w_if(x,
y), E_if(x, y), m_eff(y), p) + gamma_2;
gamma_4 = inter_scatter_emit(E_kin, h_bar, KB_J, T, D_if(x, y), Z_if(x, y), w_if(x,
y), E_if(x, y), m_eff(y), p) + gamma_3;
% Gamma --> L
y = 3;
gamma_5 = inter_scatter_abs(E_kin, h_bar, KB_J, T, D_if(x, y), Z_if(x, y), w_if(x,
y), E_if(x, y), m_eff(y), p) + gamma_4;
gamma_6 = inter_scatter_emit(E_kin, h_bar, KB_J, T, D_if(x, y), Z_if(x, y), w_if(x,
y), E_if(x, y), m_eff(y), p) + gamma_5;

% Plot the scattering rates
figure;
semilogy(E_kin / q, gamma_1, 'LineWidth', 2);
hold on;
semilogy(E_kin / q, gamma_2, 'LineWidth', 2);
semilogy(E_kin / q, gamma_3, 'LineWidth', 2);
semilogy(E_kin / q, gamma_4, 'LineWidth', 2);
semilogy(E_kin / q, gamma_5, 'LineWidth', 2);
semilogy(E_kin / q, gamma_6, 'LineWidth', 2);
```

```
hold off;

xlabel('Electron Kinetic Energy (eV)');
ylabel('Scattering Rate (1/s)');
title('Scattering Rates vs. Electron Energy (GaAs, \Gamma valley)');
legend('Acoustic', 'POP', 'gamma_X_abs', 'gamma_X_emit', 'gamma_L_abs',
'gamma_L_emit');
ylim([1e11 1e15]);
grid on;
```



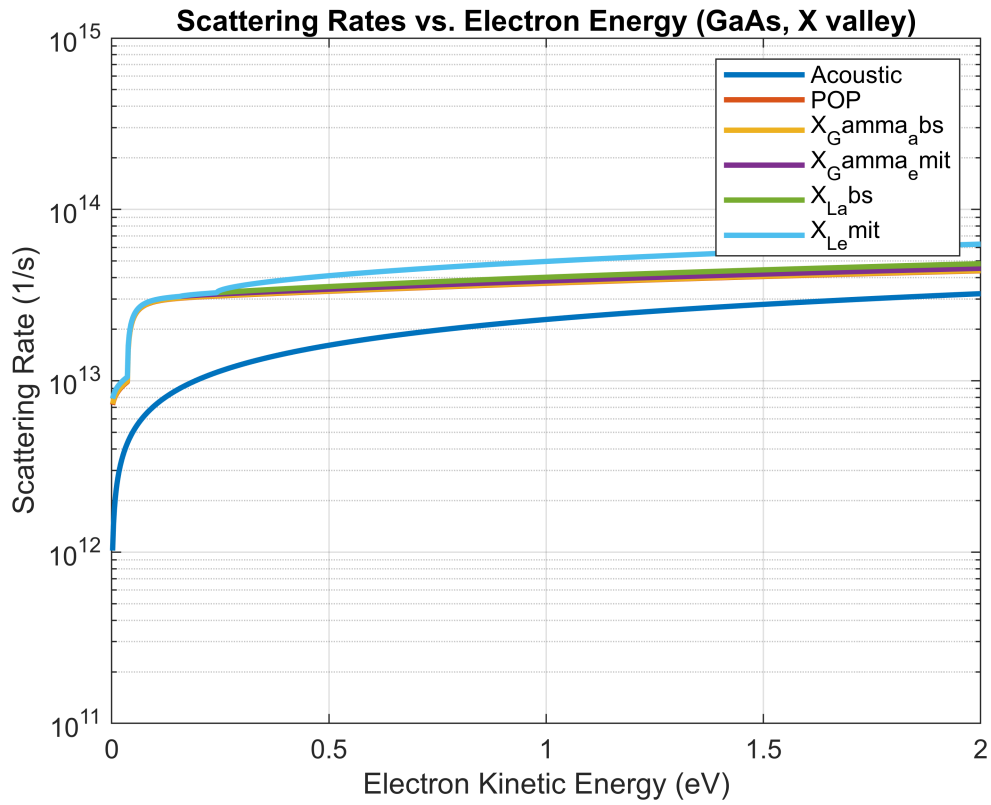
X Scattering

```
x = 2;
X_1 = ac_scatter(E_kin, m_eff(x), h_bar, p, v_s, D0(x), KB_J, T);
X_2 = scatter_pop(E_kin, m_eff(x), h_bar, w_LO, E_phonon, KB_J, q, e_inf, e_s, e_0,
T) + X_1;
% X --> Gamma
y = 1;
X_3 = inter_scatter_abs(E_kin, h_bar, KB_J, T, D_if(x, y), Z_if(x, y), w_if(x, y),
E_if(x, y), m_eff(y), p) + X_2;
X_4 = inter_scatter_emit(E_kin, h_bar, KB_J, T, D_if(x, y), Z_if(x, y), w_if(x, y),
E_if(x, y), m_eff(y), p) + X_3;
% X --> L
y = 3;
X_5 = inter_scatter_abs(E_kin, h_bar, KB_J, T, D_if(x, y), Z_if(x, y), w_if(x, y),
E_if(x, y), m_eff(y), p) + X_4;
```

```
X_6 = inter_scatter_emit(E_kin, h_bar, KB_J, T, D_if(x, y), Z_if(x, y), w_if(x, y),
E_if(x, y), m_eff(y), p) + X_5;

% Plot the scattering rates
figure;
semilogy(E_kin / q, X_1, 'LineWidth', 2);
hold on;
semilogy(E_kin / q, X_2, 'LineWidth', 2);
semilogy(E_kin / q, X_3, 'LineWidth', 2);
semilogy(E_kin / q, X_4, 'LineWidth', 2);
semilogy(E_kin / q, X_5, 'LineWidth', 2);
semilogy(E_kin / q, X_6, 'LineWidth', 2);
hold off;

xlabel('Electron Kinetic Energy (eV)');
ylabel('Scattering Rate (1/s)');
title('Scattering Rates vs. Electron Energy (GaAs, X valley)');
legend('Acoustic', 'POP', 'X_Gamma_abs', 'X_Gamma_emit', 'X_L_abs', 'X_L_emit');
ylim([1e11 1e15]);
grid on;
```



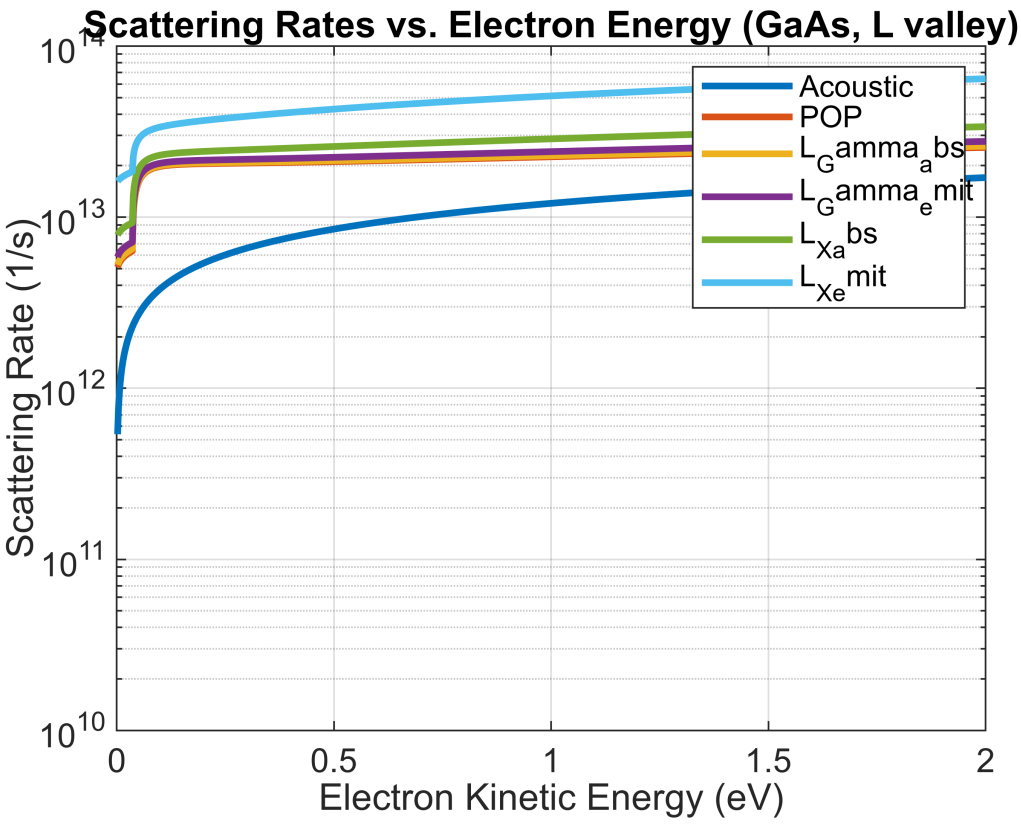
L Scattering

```
x = 3;
L_1 = ac_scatter(E_kin, m_eff(x), h_bar, p, v_s, D0(x), KB_J, T);
L_2 = scatter_pop(E_kin, m_eff(x), h_bar, w_LO, E_phonon, KB_J, q, e_inf, e_s, e_0,
T) + L_1;
```

```
% L --> Gamma
y = 1;
L_3 = inter_scatter_abs(E_kin, h_bar, KB_J, T, D_if(x, y), Z_if(x, y), w_if(x, y),
E_if(x, y), m_eff(y), p) + L_2;
L_4 = inter_scatter_emit(E_kin, h_bar, KB_J, T, D_if(x, y), Z_if(x, y), w_if(x, y),
E_if(x, y), m_eff(y), p) + L_3;
% L --> X
y = 2;
L_5 = inter_scatter_abs(E_kin, h_bar, KB_J, T, D_if(x, y), Z_if(x, y), w_if(x, y),
E_if(x, y), m_eff(y), p) + L_4;
L_6 = inter_scatter_emit(E_kin, h_bar, KB_J, T, D_if(x, y), Z_if(x, y), w_if(x, y),
E_if(x, y), m_eff(y), p) + L_5;

% Plot the scattering rates
figure;
semilogy(E_kin / q, L_1, 'LineWidth', 2);
hold on;
semilogy(E_kin / q, L_2, 'LineWidth', 2);
semilogy(E_kin / q, L_3, 'LineWidth', 2);
semilogy(E_kin / q, L_4, 'LineWidth', 2);
semilogy(E_kin / q, L_5, 'LineWidth', 2);
semilogy(E_kin / q, L_6, 'LineWidth', 2);
hold off;

xlabel('Electron Kinetic Energy (eV)');
ylabel('Scattering Rate (1/s)');
title('Scattering Rates vs. Electron Energy (GaAs, L valley)');
legend('Acoustic', 'POP', 'L_Gamma_abs', 'L_Gamma_emit', 'L_X_abs', 'L_X_emit');
ylim([1e10 1e14]);
grid on;
```


Scattering Rates vs. Electron Energy (GaAs, L valley)
Scattering Rate (1/s)
Electron Kinetic Energy (eV)
Acoustic
POP
L_Gamma_abs
L_Gamma_emit
L_Xabs
L_Xemit