

Transport Theory#1

Kinetic Theory

Kinetic theory is a formalism for describing the motion of a population of “free” particles in a solid in response to an externally applied force, such as an electric field

Key Assumptions:

- All energy and momentum is transferred by the particles in motion.
- In a statistical sense each particle is its own subsystem, i.e., the particles are fully distinguishable from each other, and are in quasi-equilibrium with temperature bath.
- Collisions are instantaneous events that randomize particle motion.

Features of Kinetic Theory:

- 1) Can define fluxes, each one being defined as the amount of some physical quantity crossing a unit area per unit time.
 - Particle flux: $\vec{J}_n = n \cdot \vec{v}$, where n is the particle density and v is the velocity. Both of these quantities are possibly functions of time and position.
 - Charge flux: $\vec{J}_q = n \cdot q \cdot \vec{v}$ (also called the electrical current)
 - Energy flux $\vec{J}_U = n \cdot [(1/2)mv^2] \vec{v}$, since all the energy is kinetic
- 2) Clearly, the particle velocity vector is very important in kinetic theory. In a first analysis, it is usually determined by classical mechanics. For example, in one dimension, we can solve for v_x from Newton's law

$$F_x = ma_x = m \frac{dv_x}{dt} \text{ where } a_x \text{ is the } x \text{ component of acceleration.}$$

For an electron in a uniform electric field, the mechanical force is $F_x = eE_x$.

So,
$$eE_x = m \frac{dv_x}{dt} \Rightarrow v_x = \frac{eE_x}{m} t + v_0, \text{ where } v_0 \text{ is the initial velocity.}$$

- 3) Clearly, a velocity increase with time cannot persist forever. It will be interrupted by collisions that can be modeled as a damping (scattering) term in *Newton's equation*.

$$\frac{mdv_x}{dt} + \frac{mv_x}{\tau} = eE_x \tag{1}$$

This is a linear 1st order inhomogeneous differential equation with constant coefficients. The solution is the sum of a homogeneous solution (setting $eE_x = 0$) and a particular solution.

Taking the initial conditions once again as $v(t=0) = v_0$, we get

$$v = \underbrace{v_0 e^{-t/\tau}}_{\text{Homogeneous}} + \underbrace{\frac{e\tau(E)}{m} (1 - e^{-t/\tau})}_{\text{Particular}}$$

- The homogeneous solution is transient and vanishes for long time scales $t \gg \tau$.
- The particular solution has a steady state term for long time scales of

$$v \rightarrow \frac{e\tau E}{m} \equiv \mu E$$

where μ is the mobility.

- Using the kinetic flux for electric current, we get

$$J_q = nqv = \frac{ne^2\tau E}{m} \equiv \sigma E \quad (\text{Ohm's Law !})$$

Where σ is called the electrical conductivity $\equiv \frac{ne^2\tau}{m}$.

Transport conductivities usually connect a given transport flux to the spatial gradient of some macroscopic potential that arises from the non-equilibrium condition. The gradients vanish in equilibrium.

For example: the charge flux is $\vec{J}_q = \sigma \vec{E} = -\sigma (\vec{\nabla} \phi)$, $\phi \rightarrow$ electrostatic potential

Similarly, the kinetic energy flux can be written

$$\vec{J}_U = -K \vec{\nabla} T$$

where T is the temperature and K is the thermal conductivity. This makes sense because heat is just the macroscopic representation of kinetic energy at the microscopic level.

Physical Interpretation of τ

- From Newton's equation, $1/\tau$ is the rate at which the initial velocity changes to the steady-state value. This certainly makes sense for a continuum ("jellium") model of the particles

under transport, and has its historic roots in fluid mechanics.

- But in the corpuscular view, we need to think about an ensemble of particles, each of which *occasionally* undergoes a randomizing collision. If we focus on a subset of the ensemble having a common velocity v_0 , then $1/\tau$ is the rate at which electrons scatter out of this subset. If the number of particles in the subset is n , we can write

$$\frac{dn}{dt} = -\frac{1}{\tau}n(t) \Rightarrow n = n_0 e^{-t/\tau}$$

Kinetic Theory and Collision Statistics

The introduction of the relaxation term in the equation-of-motion (1) is also consistent with the collision process being inherently random (i.e., stochastic). Specifically, the probability that a particle undergoes a collision in any infinitesimal time interval of length dt (between t and $t + dt$) is given by dt/τ , *independent of the time interval chosen*. This implies that the probability of a particle *not* having a collision between t and $t + dt$ is simply $1 - dt/\tau$. Thus if we define $f(t)$ as the probability of the particle *not* having a collision between 0 & t ,ⁱ we can write

$$f(t + dt) = \underbrace{\left(1 - \frac{dt}{\tau}\right)}_{\text{multiplicative probabilities}} \cdot f(t)$$

or

$$f(t + dt) - f(t) = \frac{-dt \cdot f(t)}{\tau}$$

or

$$df = -dt \frac{f(t)}{\tau}$$

or

$$\frac{df}{dt} = \frac{-f(t)}{\tau} \text{ or } \frac{df}{dt} + \frac{f(t)}{\tau} = 0$$

The solution becomes

$$f = f_0 e^{-\alpha(t)}$$

ⁱ This is synonymous with the probability of the particle going collisionless, or *ballistic*.

So if we apply the initial condition: $f(t=0)=1$, we get

$$f(t) = e^{-t/\tau} \quad (2)$$

We can now calculate the probability $P(t, \delta t)$ that an electron suffers a single collision between time t and $t + \delta t$,

$$P(t, \delta t) = \exp[-t/\tau] \cdot \delta t/\tau$$

where the first term on the right side is the probability that the particle goes without collision up to time t , and the second term is the probability that a collision occurs between t and $t + \delta t$. This $P(t, \delta t)$ has all the properties of a bonafide probability density function (pdf). For example, it is normalized,

$$\lim_{\delta t \rightarrow 0} \left\{ \int_0^\infty P(t, \delta t) dt \right\} = \int_0^\infty P(t, dt) = \int_0^\infty \frac{\exp[-t/\tau]}{\tau} dt = \frac{-\tau}{\tau} \exp[-t/\tau] \Big|_0^\infty = 1.$$

Using this pdf and integration by parts we can calculate the “mean time of survival” or, equivalently, the average time between collisions,

$$\langle t \rangle = \int_0^\infty t \cdot P(t) dt = \int_0^\infty \frac{t \cdot \exp[-t/\tau]}{\tau} dt = \langle \tau \rangle$$

This justifies our labeling of τ as the mean time between collisions.

Of greater interest is the probability $P_N(t + \delta t)$ that an ensemble of electrons suffers N collisions in a time between t and $t + \delta t$. In the same spirit as the previous derivation, this time interval can be subdivided into intervals 0 to t , and t to $t + \delta t$. If δt is small enough, then only two different outcomes can occur during this interval. Either N electrons scatter during t and none during $t + \delta t$, or $N-1$ electrons scatter during t and 1 scatters during $t + \delta t$.

Mathematically, this can be written as

$$P_N(t+\delta t) = P_N(1 - \delta t/t) + P_{N-1}(\delta t/t)$$

where $(1 - \delta t/t)$ is the probability that no collisions occur during δt , and $\delta t/t$ is the probability for a single collision in this time. This equation can be re-arranged to yield

$$\frac{P_N(t + \delta t) - P_N(t)}{\delta t} + \frac{P_N(t)}{\tau} = \frac{P_{N-1}}{\tau}$$

which can be thought of as a recursion relation relating P_N to P_{N-1} . In the limit that $\delta t \rightarrow 0$, the far-left time becomes a derivative and we get the inhomogeneous, first-order, ordinary differential equation

$$\frac{dP_N(t)}{dt} + \frac{P_N(t)}{\tau} = \frac{P_{N-1}}{\tau} \quad (3)$$

This is an important equation of probability theory and leads to the Poisson density function, as shown next.

Derivation of Poisson statistics in kinetic collisions.

Using the technique of an integrating factor and the initial condition $P_N(t = 0) = 0$, one finds the following solution to the differential Eqn (3):ⁱⁱ

$$P_N(t) = \frac{\exp(-t/\tau)}{\tau} \int_0^t \exp(t'/\tau) \cdot P_{N-1}(t') dt' \quad (4)$$

where t' is a dummy variable of integration. Fortunately, we already know the solution to this for $N = 0$, i.e., from Eqn (2), $P_0(t) \equiv f(t) = \exp(-t/\tau)$. Substitution of this into Eqn (4) yields

ⁱⁱ W.E. Boyce and R.C. DiPrima, "Elementary Differential Equations and Boundary Value Problems," 2nd Ed., (Wiley, New York, 1969, Sec. 2.1.

$$P_1(t) = \frac{t}{\tau} \exp(-t/\tau)$$

Substitution of this back into (4) and iterating yields

$$P_2(t) = \frac{1}{2} \left(\frac{t}{\tau} \right)^2 \exp(-t/\tau)$$

By logical deduction, the solution for an arbitrary number N has the form

$$P_N(t) = \frac{(t/\tau)^N}{N!} \exp(-t/\tau)$$

This is the famous Poisson density function of probability theory. Like all bonafide pdfs, it approaches a Gaussian in the limit of large samples, in this case the limit of large N. This limiting behavior is well known in probability theory through the central limit theorem. It leads to the prediction that in a solid sample having a large number of charge carriers, one expects the collision rate to fluctuate about some mean value with Gaussian statistics. This can usually be associated with a Gaussian fluctuation in the electrical conductivity of the sample: a fundamental result of fluctuation theory known as the Johnson-Nyquist theorem. The resulting Gaussian fluctuations in the open-circuit voltage or short-circuit current through electrical contacts on the sample is a phenomena of paramount importance in solid-state electronics known as Johnson-Nyquist noise.

AC Behavior of Carriers in Kinetic Theory

To understand the response of charged particles in motion to time-varying external electric fields, we go back and re-write the Newton equation of motion in terms of the instantaneous position of each particle x . We do this because it allows us to develop expressions for the *electrodynamic* response in the same physical terms as for electrostatics,

namely in terms of a dipole moment or an electrical susceptibility. Since $v \equiv dx/dt$, we can re-write (1) as

$$m(\ddot{x} + \dot{x}/\tau) = eE \quad (5)$$

We solve this for the special case of sinusoidal time-varying field, for which we can apply the phasor form $E = E_0 e^{-j\omega t}$ and write the position variable as $x = x_0 e^{-j\omega t}$. Substitution into (5) yields,

$$x = \frac{eE}{m(-\omega^2 - j\omega/\tau)}$$

From the general (electrostatic) definition, the dipole moment is $p = qx$ and

$$p = \frac{e^2 E}{m(-\omega^2 - j\omega/\tau)}$$

Again from electrostatics, the electric susceptibility is defined by $\chi_e \equiv P/(\epsilon_0 E)$, where P is the macroscopic polarization given by $P = np$. Hence, we can write

$$\chi_e = \frac{-ne^2}{m\epsilon_0(\omega^2 + j\omega/\tau)} \rightarrow \infty \quad (6)$$

This has two interesting properties: First, it diverges to infinity as $\omega \rightarrow 0$ (electrostatic limit), which makes sense physically. Since the carriers are “free”, they undergo large displacement in the electric field, limited only by the size of the solid sample. In the present analysis, this size was not constrained, so the susceptibility should diverge ! Second, it is always negative, meaning that the free-electron response is truly “dia”-electric.

When $\omega\tau \ll 1$, Eqn (6) can be re-written in a useful approximate form

$$\chi_e = \frac{ne^2}{m\varepsilon_0(-\omega^2 - j\omega/\tau)} = \frac{ne^2\tau(j)}{m\varepsilon_0\omega(1 - j\omega\tau)} \quad (7)$$

Using kinetic definition of conductivity $\sigma_0 = \frac{ne^2\tau}{m}$, we can write

$$\chi = \frac{j\sigma_0}{\varepsilon_0\omega(1 - j\omega\tau)} = \frac{j\sigma_{ac}}{\varepsilon_0\omega}$$

$$\sigma_{ac} = \frac{\sigma_0}{1 - j\omega\tau}$$

When $\omega\tau \gg 1$, (6) can be re-written in the useful form and then approximated as:

$$\chi_e = \frac{-ne^2(\omega - j/\tau)}{m\omega\varepsilon_0(\omega^2 + 1/\tau^2)} = \frac{-\tau\omega_p^2(\omega\tau - j)}{\omega(\omega^2\tau^2 + 1)} \approx \frac{-\omega_p^2}{\omega^2} + j\frac{\omega_p^2}{\omega^3\tau} \quad (8)$$

where ω_p is the plasma frequency $\omega_p = (ne^2/m\varepsilon_0)^{1/2}$. Now, since $\varepsilon \equiv 1 + \chi_e$, we can write

$$\varepsilon \approx 1 - \frac{\omega_p^2}{\omega^2} + j\frac{\omega_p^2}{\omega^3\tau} \approx 1 - \frac{\omega_p^2}{\omega^2} \quad (9)$$

This leads to the oft-made statement that the dielectric constant of metals is large and negative up to the plasma frequency, where it rapidly drops to about unity. Of course, this statement requires $\omega\tau > 1$ and completely ignores the atomic and ionic polarizability contributions, which can often be added independently of the free-electron response.

Eqns (7), (8), and (9) are extremely useful in the analysis of metals, semimetals, and semiconductors. To determine when each is applicable we need to know that for bulk gold,

$\tau \cong 3 \times 10^{-14}$ sec and $n = 5.9 \times 10^{22} / \text{cm}^{-3}$. This leads to $\omega_p = 1.37 \times 10^{16} \text{ s}^{-1}$ (gold) and

$$f_p = 2.18 \times 10^{15} \text{ s}^{-1} \text{ or } \lambda_p = c / f_p = 0.138 \mu\text{m}$$

, which is well into the ultraviolet portion of the

spectrum. Similarly, we can define a scattering circular frequency by $\omega_s = 1/\tau$, or $\omega_s =$

$3.3 \times 10^{13} \text{ s}^{-1}$, or $f_s = 5.3 \times 10^{12} \text{ s}^{-1}$. So in the near-infrared and visible regions, we have $\omega\tau \gg 1$.

The overall behavior of Eqns (6), (7), and (8) is represented by the qualitative plot

given below with:

$$\text{Re}\{\chi_e\} = \frac{-\omega_p^2 \tau^2}{1 + \omega^2 \tau^2} \quad \text{and} \quad \text{Im}\{\chi_e\} = \frac{\omega_p^2 \tau}{\omega(1 + \omega^2 \tau^2)}$$

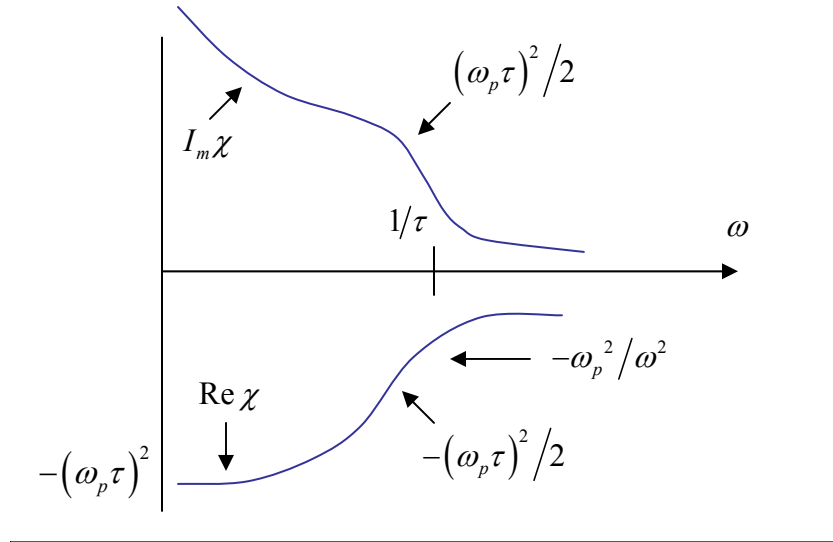


Fig. 1. Real and imaginary parts of χ_e vs frequency. Note: at $\omega = 1/\tau$, $|\text{Re}\{\chi_e\}| = |\text{Im}\{\chi_e\}|$

Motion in a Magnetic Field

We go back and generalize *Newton's equation* for particle velocity in the presence of a *Lorentz force* in a magnetic field. We must keep track of vectors and signs.

$$m \frac{d\vec{v}}{dt} + \frac{m\vec{v}}{\tau} = q(\vec{E} + \vec{v} \times \vec{B})$$

$q \rightarrow$ - sign (electron), + sign (hole)

$$q(\vec{v} \times \vec{B}) \rightarrow \text{Lorentz force} = -e \left(\vec{v} \times \vec{B} \right) \rightarrow \text{for electron}$$

In general the *Lorentz term* complicates the solution greatly unless $\vec{B}$ is uniform. Let's assume $\vec{B} = B_0 \hat{z}$, and write general form $\vec{v} = v_x \hat{x} + v_y \hat{y} + v_z \hat{z}$.

So,

$$\vec{v} \times \vec{B} = -v_x B_0 \hat{y} + v_y B_0 \hat{x}$$

Matching cartesian components on both sides, we get

$$\begin{aligned} \hat{x} : m \frac{dv_x}{dt} + \frac{mv_x}{\tau} &= qE_x + qv_y B_0 \\ \hat{y} : m \frac{dv_y}{dt} + \frac{mv_y}{\tau} &= qE_y - qv_x B_0 \\ \hat{z} : m \frac{dv_z}{dt} + \frac{mv_z}{\tau} &= qE_z \end{aligned}$$

Again, each equation is a 1st order linear, inhomogeneous differential equation having both a homogeneous and a particular solution:

$$\begin{aligned} v_x &= v_{0x} e^{-t/\tau} + \frac{q}{e} \frac{e\tau}{m} (E_x + v_y B_0) (1 - e^{-t/\tau}) \\ v_y &= v_{0y} e^{-t/\tau} + \frac{q}{e} \frac{e\tau}{m} (E_y - v_x B_0) (1 - e^{-t/\tau}) \\ v_z &= v_{0z} e^{-\frac{t}{\tau}} + \frac{q}{e} \frac{e\tau}{m} E_z (1 - e^{-t/\tau}) \end{aligned}$$

The key result of the *Lorentz force* is that it couples components of velocity lying in the plane perpendicular to $\vec{B}$. In the steady state and for $t \gg \tau$.

$$\begin{aligned} v_x &\rightarrow (\mu E_x + \omega_c \tau v_y) \frac{q}{e} \\ v_y &\rightarrow (\mu E_y - \omega_c \tau v_x) \frac{q}{e} \\ v_z &\rightarrow \mu E_z \left(\frac{q}{e} \right) \end{aligned}$$

where $\omega_c \equiv eB_0/m$ is called the *cyclotron frequency* (a ubiquitous constant in magneto-transport problems, much like the Larmor frequency and Bohr magneton occur in magnetostatic problems). Suppose the lateral extent of a sample is finite along y and z axes, and an electric field E_x is applied along $\hat{x}$. In steady state, v_y and v_z must be zero if charge carriers are confined to sample. This reasoning leads to:

$$\begin{aligned} v_z = 0 &\Rightarrow E_z = 0 \\ v_y = 0 &\Rightarrow \mu E_y = \omega_c \tau v_x \end{aligned} \quad (6)$$

and

$$v_x = \left(\frac{q}{e} \right) \mu E_x \text{ (as expected)}$$

Eqn (6) implies

$$E_y = \frac{\omega_c \tau}{\mu} v_x = \frac{q}{e} \omega_c \tau E_x = q \frac{B_0 \tau}{m} E_x$$

$\uparrow$
Linear in v_x

$\uparrow$
Linear in B

The linear dependence on v_x is consistent with experimental observation of linear dependence on J_x (electrical current density). By noting that $J_x = nq v_x$ (*kinetic theory*), we get

$$E_y = \left(q \frac{B_0}{m} \right) (\tau) \left(\frac{e}{q} \right) \left(\frac{m}{e\tau} \right) \frac{J_x}{nq} = \frac{B_0 J_x}{nq} ; \text{ a famous result called the } \textit{Hall effect}.$$

The ratio $\frac{E_y}{B_0 J_x} = \frac{1}{nq}$ is called the *Hall Coefficient for electrons* $\equiv R_H$

$R_H \rightarrow$ negative for electrons (or any negatively charged particles), and positive for holes (or any positively charged particles). Note: R_H does not depend on mass (or effective mass).

The *Hall effect* is very important historically and in modern technology as well.

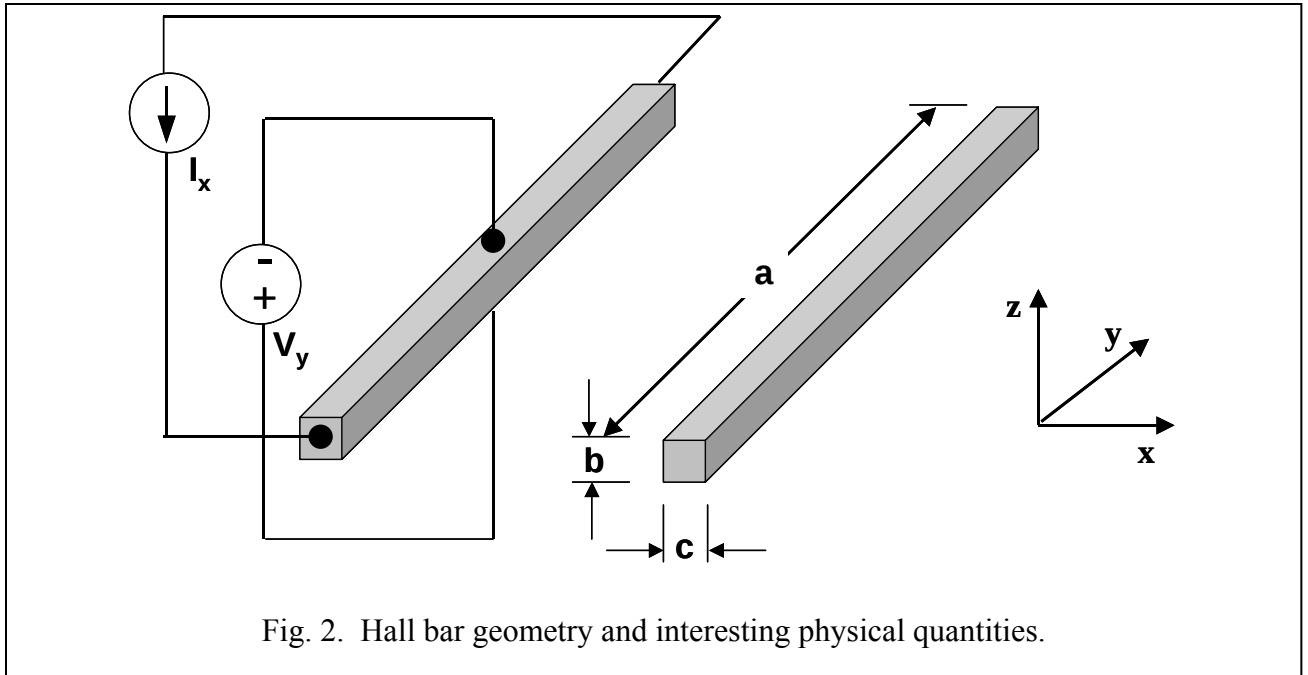
Hall Effect Example (Hall Bar)

Fig. 2. Hall bar geometry and interesting physical quantities.

We know for the geometry in Fig. 2 that if the external electric field is applied along the x axis and external magnetic field is applied along the z axis, then there will be a response

electric field along y axis given by $E_y = \frac{B_0 J_x}{nq}$ where J_x is the current density and n is the

mobile charge density. But if current is uniform $J_x = \frac{I_x}{A} = \frac{I_x}{b \cdot c}$. And if E_y is

uniform, $E_y = \frac{V_y}{b}$, so we get

$$\frac{V_y}{b} = \frac{B_0 I_x}{nqbc}$$

or

$$V_y = \frac{B_0 I_x}{nqc}$$

For example, let's take a Si Hall bar having $n = 1 \times 10^{16} / \text{cm}^3 = 1 \times 10^{22} / \text{m}^3$

↑
electrons

Suppose $B_0 = 1 \text{ T}$ (10 KG), $I_x = 1 \text{ mA}$; and $c = 1 \text{ mm}$

$$\Rightarrow V_y = \frac{(1)(0.001)}{10^{22}(-1.6 \times 10^{-19})(10^{-3})} = -0.62 \text{ mV}$$

Minus sign for electrons

Minus signs means E_y is pointing opposite to $\hat{y}$

In contrast, gold has $n = 5.9 \times 10^{22} / \text{cm}^3 = 5.9 \times 10^{28} / \text{m}^3$. So,

$$|R_H| = \frac{1}{ne} = 1.06 \times 10^{-10} \text{ m}^3 / \text{Cb}$$

A more interesting quantity physically is the ratio of $E_y/E_x = \omega_c \tau$.

For pure bulk gold, $\tau \approx 30 \text{ fs}$, so that $\frac{\omega_c}{B} = \frac{e}{m} = 1.76 \times 10^{11} \text{ s}^{-1} / \text{T}$

Let $B_0 = 1 \text{ T} \Rightarrow \omega_c = 1.76 \times 10^{11}$, $\omega_c \tau = 0.005$, $E_y/E_x = 0.005$

In semiconductors, E_y/E_x becomes much larger for two reasons:

- (1) $\omega_c/B = e/m \rightarrow e/m^*$ increases greatly since $m^* \ll m_e$
- (2) τ increases by one order of magnitude over that in metals (typically).