



UNIVERSITY OF STRASBOURG

Tutorial II

Semi-Classical Electron Transport in Metals

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1 Optional reminder

In the interest of time, the derivations in this Section won't be performed in details during the class. Rather, we will briefly review the main results that will be useful to address Section 2 and discuss their physical meaning.

1.1 Semi-classical dynamics

We consider an electron in a one-dimensional periodic potential $\mathcal{V}(x)$, with period a . Its wavefunction can be expressed in the Bloch form :

$$\Psi(k, x) = u(k, x)e^{ikx}, \quad (1.1)$$

where $\hbar k$ is the electron quasi-momentum (a.k.a. crystal momentum) and $u(k, x)$ has the same spatial periodicity as $\mathcal{V}(x)$. The eigenenergies of the Hamiltonian $\mathcal{H} = p^2/2m + \mathcal{V}(x)$ are denoted $\mathcal{E}(k)$, with p and m , the momentum operator and free electron mass, respectively.

- i — Express the electron semi-classical velocity $v(k) = \langle \Psi(k, x) | \frac{p}{m} | \Psi(k, x) \rangle$ as a function of $\mathcal{E}(k)$.

We can consider a Bloch wavefunction in 1D,

$$\psi(k, x) = u(k, x)e^{ikx}$$

the electrons are experiencing a potential, with this, we can express the semi-classical velocity v ,

$$v = \langle \psi(k, x) | \frac{p}{m} | \psi(k, x) \rangle$$

where $p = -i\hbar\partial_x$, and thus,

$$\mathcal{E}(k) \equiv \langle \psi | \mathcal{H} | \psi \rangle = \langle \psi | \frac{p^2}{2m} + V(x) | \psi \rangle$$

and we can write the same thing using the Bloch wavefunction explicitly instead of ψ ,

$$\mathcal{E}(k) = \langle u | \frac{(p + \hbar k)^2}{2m} + V(x) | u \rangle$$

and now if we derivate this expression,

$$\frac{d}{dk}\mathcal{E}(k) = \frac{d}{dk} \left(\langle u | \frac{(p + \hbar k)^2}{2m} + V(x) | u \rangle \right)$$

But, we know that, $\langle \psi_k | \dots | u \rangle = \langle u | \dots | \partial_k u \rangle = 0$, leading to,

$$v(k) = \frac{1}{\hbar} \frac{d\mathcal{E}(k)}{dk}$$

- ii — We now apply an external electric field E_0 . Express the rate of change of electron quasi-momentum. This result is known as the *acceleration theorem*.

If we apply an external field E_0 , we get that,

$$d\mathcal{E} = -eE_0vdt$$

leading us to,

$$\frac{d\hbar k}{dt} = -eE_0$$

which is the so-called *acceleration theorem*.

- iii — Using the expression of $v(k)$, write down the equation of motion of an electron in a Newton-like form and define the effective mass m^* .

$$\frac{dv}{dt} = \frac{1}{\hbar} \frac{d}{dt} \frac{d\mathcal{E}(k)}{dk} = \frac{1}{\hbar} \frac{d^2\mathcal{E}(k)}{dk^2} \frac{dk}{dt}$$

Using the acceleration theorem,

$$m^* \frac{dv}{dt} = -eE_0$$

with m^* the effective mass defined as,

$$\frac{1}{m^*} = \frac{d^2\mathcal{E}(k)}{dk^2}$$

- iv — We now consider the Hamiltonian $\mathcal{H} = p^2/2m + \mathcal{V}(x) + eE_0x$, where e is the elementary charge. At $t = 0$, the electron is prepared in a Bloch state $\Psi(k_0, x)$. Show that the time-dependent wavefunction $\Psi(x, t; E_0)$ obeys :

$$\Psi(x + A, t; E_0) = e^{ik(t)a} \Psi(x, t; E_0), \quad (1.2)$$

where

$$k(t) = \frac{1}{\hbar} eE_0t + k_0. \quad (1.3)$$

Connect this result to the previous question.

- v — Discuss the physical meaning and peculiarities of the semi-classical velocity and effective mass in the case of an electronic band $\mathcal{E}(k)$ with a) parabolic and b) linear dispersion.

Near a band edge, $v(k)$ goes to 0. If you take linear dispersion, you have a divergence of the effective mass (we will talk more on that on the physics of graphene of the next exercise sheet).

1.2 The Drude model

In this section, we connect the electron current density $\mathbf{J}(\mathbf{r}, t)$ to an applied electric field $\mathbf{E}(\mathbf{r}, t)$. In the linear response theory, these two vectors are linked by a conductivity tensor $\sigma_{\alpha,\beta}$, with $\alpha, \beta = x, y, z$, and the response is a priori non-local. Introduced by Paul Drude in 1900, the classical, phenomenological Drude model provides a simple and intuitive expression of the frequency dependent conductivity. In spite of its inherent limitations, the Drude model is an excellent introduction to electron transport in metals.

- i — Let us consider a metal with a density of independent and free electrons, denoted n . A spatially uniform electric field \mathbf{E} is applied. The conduction electrons undergo collisions at a rate τ^{-1} , that are independent of their position and velocity. After a collision, the electron velocity is a random vector. Establish the classical equation of motion for a single electron.

$$m \frac{d\vec{v}}{dt} = -m \frac{\vec{v}}{\tau} - e\vec{E}_0$$

- ii — We first consider the stationary regime, $\mathbf{E}(\mathbf{r}, t) = \mathbf{E}_0$. Express the current density $\mathbf{J} = -ne\mathbf{v}$ and deduce the static conductivity σ_0 . Provide (and justify) an order of magnitude estimate for τ , n , and σ_0 .

In the static regime,

$$\vec{j} = \sigma \vec{E}_0, \quad \sigma = \frac{ne^2\tau}{m}$$

nothing but the Lorentz model if we clip the string. τ is of the order of ns to few fs. The typical density in copper is $n_{\text{Cu}} \sim 9.5 \times 10^{28} \text{ cm}^3$.

- iii — We consider a uniform harmonic field $\mathbf{E}_0 e^{-i\omega t}$ that oscillates at the angular frequency ω . Express the frequency dependent conductivity $\sigma(\omega)$.

$$\vec{E} = \vec{E}_0 e^{-i\omega t}$$

we can inject in the same equation of motion thus leading to

$$\sigma(\omega) = \frac{\sigma_0}{1 - i\omega\tau}$$

which is the so-called *frequency dependent conductivity* (still a local quantity, in principle σ depends on q and ω with $\vec{E} = \vec{E}_0 e^{i(\vec{q} \cdot \vec{r} - \omega t)}$: \vec{q} is the incoming wavevector). This expression is like a low-pass filter.

iv — Calculate $\langle \mathbf{J} \cdot \mathbf{E} \rangle$, the time-averaged dissipated power per unit volume and comment this result.

Dissipated power

$$\mathcal{P} = \langle \vec{J} \cdot \vec{E} \rangle = \sigma_1(\omega) \langle |\vec{E}|^2 \rangle$$

with $\sigma(\omega) = \sigma_1(\omega) + i\sigma_2(\omega)$. σ_1 (real part) is directly correlated to absorption.

v — The electrical conductivity is intimately related to the dielectric function $\epsilon(\omega)$ through :

$$\epsilon(\omega) = 1 + i \frac{\sigma(\omega)}{\epsilon_0 \omega}, \quad (1.4)$$

with ϵ_0 the vacuum dielectric permittivity. Give approximate expressions of the real and imaginary part of $\epsilon(\omega)$ in the three distinct regimes : a) $\omega\tau \ll 1$, b) $1 < \omega\tau \ll \omega_p\tau$, c) $\omega \approx \omega_p$ and $\omega \geq \omega_p$, where $\omega_p^2 = \frac{ne^2}{\epsilon_0 m}$ is the plasma frequency. Comment on these results.

Maxwell's equation,

$$\frac{d^2 E(z)}{dz^2} = -\frac{\omega^2}{c^2} \left[1 + i \frac{\sigma(\omega)}{\epsilon_0 \omega} \right] E(z)$$

$$\epsilon(\omega) = N^2(\omega)$$

with ϵ is the dielectric constant, N the (complex) refractive index,

$$\epsilon(\omega) = 1 + \frac{i\sigma(\omega)}{\epsilon_0 \omega}$$

Which is a direct link between conductivity and dielectric constant ($\epsilon(\omega) = \epsilon_1(\omega) + i\epsilon_2(\omega)$).

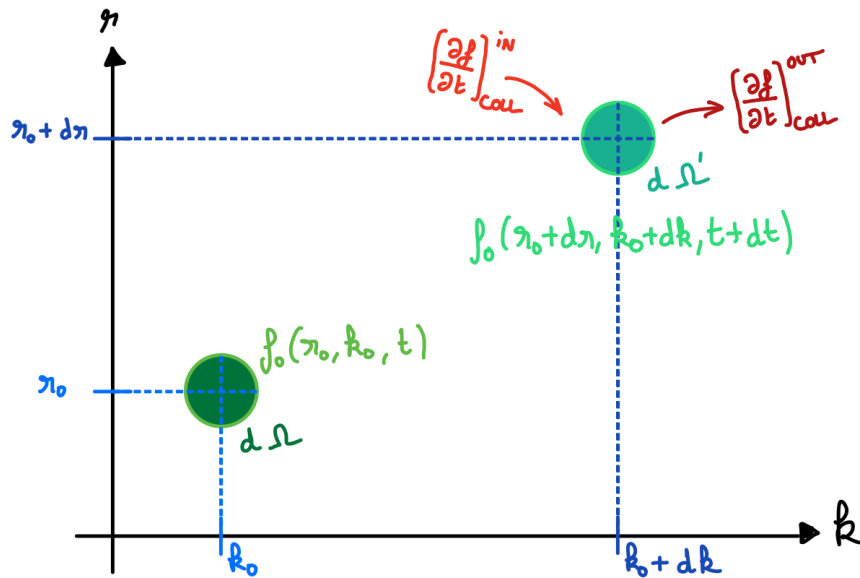
2 Static and dynamical conductivity from Boltzmann equation

The aim of this section is to derive expressions for the electronic intraband conductivity in a metal. Let us consider a single partially filled electronic band $\mathcal{E}(k)$. At thermodynamic equilibrium, the electrons follow a Fermi-Dirac distribution :

$$f_0(\mathbf{k}) = \frac{1}{e^{(\mathcal{E}(\mathbf{k}) - \mathcal{E}_F)/k_B T} + 1}, \quad (2.1)$$

with \mathcal{E}_F the Fermi energy, k_B the Boltzmann constant and T the temperature.

- i — Assuming a parabolic band with effective mass m^* , provide the expression of the Fermi wavevector k_F as a function of the electron density n and of the Fermi velocity v_F . Describe the Fermi surface.



$$\mathcal{E}(k) = \frac{\hbar k^2}{2m^*}$$

$$N = \sum_k^{k \leq k_F} g_s = 2 \frac{V}{(2\pi)^3} \frac{4}{3} \pi k_F^3$$

where g_s is the spin degeneracy taken as 2 here. k_F is the Fermi wavevector,

$$k_F^3 = 3\pi^2 n$$

with $n = N/V$.

We now aim to describe how $f_0(\mathbf{k})$ is modified into a distribution $f(\mathbf{r}, \mathbf{k}, t)$ by an external perturbation (external fields, temperature gradient,...). For this purpose, circa 1872, Ludwig Boltzmann developed a general framework that is still widely used to describe out of equilibrium processes, including transport phenomena

.In the following, we shall focus on the effect of an applied electric field \mathbf{E} to conduction band electrons in a metal. The Boltzmann transport equation writes :

$$f\left(\mathbf{r} + \mathbf{v}dt, \mathbf{k} - \frac{e\mathbf{E}}{\hbar}dt, t + dt\right) = f(\mathbf{r}, \mathbf{k}, t) + \left[\frac{\partial f}{\partial t}\right]_{\text{coll}} dt. \quad (2.2)$$

Electrons undergo collisions (with other charge carriers, phonons, impurities, structural defects,...) which for simplicity are described using the *relaxation time approximation*, such that :

$$\left[\frac{\partial f}{\partial t}\right]_{\text{coll}} = \frac{f_0(\mathbf{k}) - f(\mathbf{r}, \mathbf{k}, t)}{\tau}. \quad (2.3)$$

Assuming a *weak* perturbation, (2.2) can be expanded to first order. Using (2.3), we then obtain the simplified expression :

$$\frac{\partial f}{\partial \mathbf{r}} \cdot \mathbf{v} - \frac{e}{\hbar} \frac{\partial f}{\partial \mathbf{k}} \cdot \mathbf{E} + \frac{\partial f}{\partial t} = \frac{f_0 - f}{\tau}. \quad (2.4)$$

2.1 Static conductivity

- i — Let us consider a uniform system and assume that the field \mathbf{E} is turned off at $t = 0$. From (2.4), derive the expression of $f(\mathbf{k}, t)$.

Uniform field, meaning that the gradient of it is zero. So we end up with,

$$\frac{\partial f}{\partial t} = \frac{f_0 - f}{\tau}$$

The solution of this is just an exponential relaxation (with a timescale τ) back to the Fermi-Dirac distribution,

$$f(\mathbf{r}) = f_0 + \left[f(\vec{k}, t = 0) - f_0\right] e^{-t/\tau}$$

with $f(\vec{k}, t = 0)$ our initial condition.

- ii — We now consider a uniform static field \mathbf{E} . Derive a simplified expression of (2.4) in the form $f = f_0 + f_1$, with

$$f_1 = e\tau \frac{\partial f_0}{\partial \mathcal{E}} \mathbf{v} \cdot \mathbf{E}, \quad (1)$$

with v the semi-classical velocity introduced in Sec. 1. Draw a schematic representation of f_0 and f in the (k_x, k_y) plane, where \mathbf{E} is taken along the x axis for clarity.

We want to understand what happens under a static, uniform \vec{E} field.

$$\frac{\partial}{\partial \vec{r}} f = 0; \quad \frac{\partial f}{\partial t} = 0$$

But $\vec{E} \neq \vec{0}$, thus (2.4) reads,

$$-\frac{e}{\hbar} \frac{\partial f}{\partial \vec{k}} \cdot \vec{E} = -\frac{f_1}{\tau}$$

We want the lowest order in \vec{E} (or field strength), this implies that

$$\frac{\partial f}{\partial \vec{k}} \approx \frac{\partial f_0}{\partial \vec{k}} + \mathcal{O}(\vec{E}^2)$$

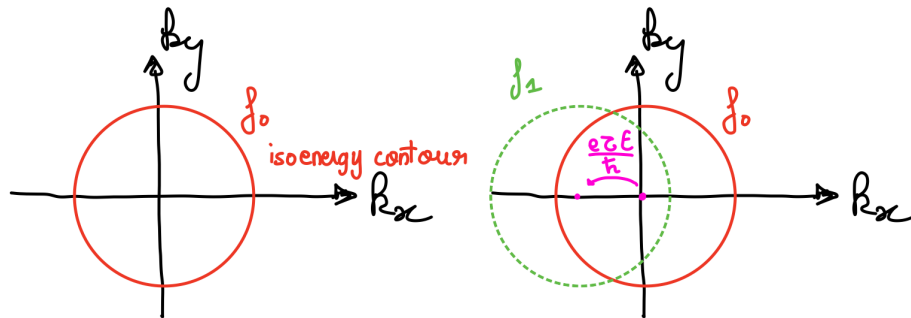
(because $\partial_{\vec{k}} f_1$ would give a contribution that depends on \vec{E}). We can just write,

$$-\frac{e}{\hbar} \frac{\partial f_0}{\partial \vec{k}} \cdot \vec{E} = -\frac{f_1}{\tau}$$

we can use $f = f_0 + f_1$,

$$f(\vec{k}) \approx f_0 \left(\vec{k} + \frac{e\tau \vec{E}}{\hbar} \right)$$

Which is a shifted Fermi-Dirac distribution by $e\tau E/\hbar$.



Orders of magnitude

$$E \sim 10^6 \text{ V.m}^{-1}, \quad \frac{\hbar}{\tau} \sim 0.1 \text{ eV}$$

we have that $e\tau E/\hbar \ll k_F$ so our approximation still hold.

- iii — We write the current density as $\mathbf{J} = -\frac{2}{(2\pi)^3} \int e\mathbf{v}f d\mathbf{k}$? Discuss this expression. Assuming an isotropic system, \mathbf{J} and \mathbf{E} are parallel and the conductivity σ_0 becomes a scalar. Show that :

$$\sigma_0 = \frac{e^2}{4\pi^3} \int \tau(\hat{\mathbf{e}} \cdot \mathbf{v})^2 \left(-\frac{\partial f_0}{\partial \mathcal{E}} \right) dk, \quad (2.6)$$

where \mathbf{E} is carried by the unit vector $\hat{\mathbf{e}}$.

$f = f_0 + f_1$ and f_0 provides no contribution to the current density. Thus,

$$\vec{J} = -\frac{2}{(2\pi)^3} \int e\vec{v} \left(e\tau \frac{\partial f_0}{\partial \mathcal{E}} \vec{v} \cdot \vec{E} \right) d\vec{k}$$

We can write $\vec{E} = E\hat{\mathbf{e}}$, thus,

$$\|\vec{J}\| = -\frac{2}{(2\pi)^3} \int d\vec{k} e^2 E \tau (\vec{v} \cdot \hat{\mathbf{e}})^2 \frac{\partial f_0}{\partial \mathcal{E}}$$

from equipartition of energy, we can write $(\vec{v} \cdot \hat{\mathbf{e}})^2 = v^2/3$.

- iv — Provide a sensible approximation for the derivative of the Fermi distribution f_0 . Using the following identity

$$\int \delta[\mathcal{E}(\mathbf{k}) - \mathcal{E}_F] \equiv \int_{\mathcal{E}(\mathbf{k})=\mathcal{E}_F} \frac{dS}{|\nabla_{\mathbf{k}} \mathcal{E}(\mathbf{k})|}, \quad (2.7)$$

demonstrate that one recovers an expression analogous to the static Drude conductivity in the case of a parabolic conduction band.

We can write $J = \sigma_0 E$, thus,

$$\sigma_0 = \frac{e^2}{12\pi^3} \int \tau v^2 \left(-\frac{\partial f_0}{\partial \mathcal{E}} \right) d\vec{k}$$

and using Eq. (2.7) and the assumption that in first approximation the derivative $\partial_{\mathcal{E}} f_0 \approx \delta$,

$$\begin{aligned} \sigma_0 &= \frac{e^2}{12\pi^3} \int_{\text{fermi sphere}} v^2 \tau \delta(\mathcal{E}(\vec{k}) - \mathcal{E}_F) d\vec{k} \\ &= \frac{e^2}{12\pi^3} \int_{\text{fermi surface}} v_F^2 \tau_F \frac{1}{\partial \mathcal{E}(k)/\partial k} d\Sigma_F \end{aligned}$$

Thus using $d\Sigma_F = k_F^2 \sin \theta d\theta d\varphi$ and $v_F = (1/\hbar) \times \partial \mathcal{E}(\vec{k})/\partial k|_{\mathcal{E}=\mathcal{E}_F}$,

$$\begin{aligned} \sigma_0 &= \frac{e^2 \tau_F}{12\pi^3} \iint_{\theta, \varphi} \frac{v_F}{\hbar} k_F^2 \sin \theta d\theta d\varphi \\ &= \frac{e^2 \tau_F}{3\pi^2} \frac{k_F^3}{m^*} \rightarrow \frac{ne^2 \tau_F}{m^*} \end{aligned}$$

which we recover Drude's model prediction.

2.2 Frequency and wavevector dependence of the conductivity

Let us now consider a harmonic *transverse* electric field $\mathbf{E} = \mathbf{E}_0 e^{i(\mathbf{q} \cdot \mathbf{r} - \omega t)}$, oscillating at the angular frequency ω and propagating along the wavevector $\mathbf{q} \perp \mathbf{E}_0$.

i — Writing, as in Sec. 2.1 $f = f_0 + f_1$, with the ansatz $f_1(\mathbf{r}, \mathbf{k}, t) = \phi(\mathbf{k}) e^{i(\mathbf{q} \cdot \mathbf{r} - \omega t)}$ and restricting the calculations to the lowest order, show that (2.4) yields :

$$\phi(\mathbf{k}) = \frac{e\tau \mathbf{v} \cdot \mathbf{E}_0}{1 - i\tau(\omega - \mathbf{q} \cdot \mathbf{v})} \frac{\partial f_0}{\partial \mathcal{E}}, \quad (2.8)$$

and express the frequency and wavevector dependent $\sigma(\mathbf{q}, \omega)$ in the case of an isotropic medium (as in Sec. 2.1 (iv)). One may verify that the frequency dependent Drude conductivity (see Sec. 1.2 (iii)) is again recovered in the long wavelength limit ($|\mathbf{q}| \rightarrow 0$).

f_0 has no contribution to the current \vec{J} , the simple idea is that this distribution is not dependent on the wave-vector, isotropic distribution in momentum-space, so if you find an electron with wavevector $\hbar \vec{k}$, you'll find an other one with $-\hbar \vec{k}$, so the contributions cancels out. If we want to restrict ourselves to first order in the field $\|\vec{E}\|$, this leads us to the assumption,

$$\frac{\partial f}{\partial \vec{k}} = \frac{\partial f_0}{\partial \vec{k}}$$

because otherwise, we would get terms that are non-linear with respect to $\|\vec{E}\|$. Boltzmann equation,

$$\frac{\partial f}{\partial \vec{r}} \cdot \vec{v} - \frac{e}{\hbar} \frac{\partial f_0}{\partial \vec{k}} \cdot \vec{E} + \frac{\partial f}{\partial t} = \frac{f_0 - f}{\tau}$$

Also, we know that f_0 is independent of \vec{r} and thus,

$$\frac{\partial f_0}{\partial \vec{r}} = 0$$

with the ansatz $f_1(\mathbf{r}, \mathbf{k}, t) = \phi(\mathbf{k}) e^{i(\mathbf{q} \cdot \mathbf{r} - \omega t)}$, Boltzmann equation yields,

$$i\vec{q} \cdot \vec{v} - \frac{e}{\hbar} \frac{\partial f_0}{\partial \vec{k}} \cdot \vec{E} + \frac{\partial f_1}{\partial t} = -\frac{f_1}{\tau}$$

And thus, using the chain rule derivation $\partial_k f_0 = \partial_{\mathcal{E}} f_0 \partial_k \mathcal{E}$,

$$\phi(\vec{k}) = \frac{e\tau \vec{v} \cdot \vec{E}_0}{1 + i\tau(\vec{q} \cdot \vec{v} - \omega)} \frac{\partial f_0}{\partial \mathcal{E}}$$

$$\vec{J} = -\frac{\tau}{(2\pi)^3} \int e\vec{v} f_1 d^3k$$

where \vec{J} depends on \vec{q} and ω .

This leads to,

$$\sigma(\vec{q}, \omega) = \frac{e^2}{4\pi^3} \int \frac{\tau v^2/3}{1 + i\tau(\vec{q} \cdot \vec{v} - \omega)} \left(-\frac{\partial f_0}{\partial \mathcal{E}} \right) d^3k$$

We introduce $s = iq\Lambda(\omega)$, where $\Lambda(\omega)$ is the frequency dependent mean free path.

We now focus on the frequent case of a parabolic energy band. We assume that the applied electric field oscillates along the x direction and propagates with a wavevector along the z direction. We admit that the following analytic expression can be obtained from a derivation similar to Sec. 2.1 (v) :

$$\sigma(q, \omega) = \frac{3}{4} \frac{\sigma_0}{1 - i\omega\tau} \left[\frac{2}{s^2} + \frac{s^2 - 1}{s^3} \ln\left(\frac{1+s}{1-s}\right) \right], \quad (2.9)$$

where $s = \frac{iqv_F\tau}{1 - i\omega\tau} \equiv iq\Lambda(\omega)$.

ii — Give a physical interpretation for $\Lambda(\omega)$.

$\Lambda(\omega)$ is the frequency dependent mean free path.

iii — Discuss and comment the two limiting cases : a) $|s| \ll 1$, b) $|s| \gg 1$.

a)

$$\Lambda \ll \frac{1}{q} = \frac{\lambda}{2\pi}$$

This is the so-called Drude (or normal) region, so we can make a Taylor expansion,

$$\left(\frac{2}{s^2} + \frac{s^2 - 1}{s^3} [\ln(1+s) - \ln(1-s)] \right) \approx \frac{4}{3}$$

we expanded to 3rd order. And thus,

$$\sigma \approx \frac{\sigma_0}{1 - i\omega\tau}$$

b)

$$\Lambda \gg \lambda$$

In that case, it would correspond to the ballistic regime,

$$\left[\frac{2}{s^2} + \frac{s^2 - 1}{s^3} \ln\left(\frac{1+s}{1-s}\right) \right] \simeq \frac{i\pi}{s}$$

$$\ln\left(\frac{1+s}{1-s}\right) = \ln(-1) + \ln\left(\frac{1+\frac{1}{s}}{1-\frac{1}{s}}\right) \approx i\pi + \mathcal{O}\left(\frac{1}{s}\right)$$

And thus now,

$$\sigma = \frac{\sigma_0\pi}{qv_F\tau}$$

What is important now is that σ depends on q and not on ω ,

$$\sigma = \sigma_0 \times \eta(q)$$

where $\eta(q)$ is a function of the conduction electrons that contribute to electronic transport. With $\eta(q) \ll 1$.

In electron with \vec{v}_F nearly parallel to \vec{q} will see a field changing $qv_F\tau$ times before a collision occurs, meaning negligible contribution to transport.

Only electrons such that \vec{v}_F is almost parallel to \vec{E}_0 will contribute. Thus we can estimate,

$$\sigma \sim \frac{\sigma_0}{qv_F\tau}$$

Note : The fact that $\sigma(q)$ is directly linked to k_F has been used to map Fermi surfaces in metals.