

THE CONDUCTIVITY TENSOR

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1. VECTOR POTENTIAL AND CURRENTS

The Hamiltonian of N identical particles with charge q minimally coupled to an assigned vector potential $\mathbf{A}(\mathbf{x}, t)$ is:

$$(1) \quad \begin{aligned} \hat{H}_{\mathbf{A}}(t) &= \sum_{i=1}^N \frac{1}{2m} (\hat{\mathbf{p}}_i - \frac{q}{c} \mathbf{A}(\hat{\mathbf{x}}_i, t))^2 + \hat{V}(\hat{\mathbf{x}}_i) + \hat{U}_{int}(\hat{\mathbf{x}}_1, \dots, \hat{\mathbf{x}}_N), \\ &= \hat{H} - \frac{q}{c} \int d\mathbf{x} \hat{\mathbf{j}}(\mathbf{x}) \cdot \mathbf{A}(\mathbf{x}, t) + \frac{q^2}{2mc^2} \int d\mathbf{x} \hat{n}(\mathbf{x}) \mathbf{A}^2(\mathbf{x}, t) \end{aligned}$$

$\hat{n}(\mathbf{x}) = \sum_{i=1}^N \delta(\mathbf{x} - \hat{\mathbf{x}}_i) = \sum_{\mu} \hat{\psi}_{\mu}^{\dagger}(\mathbf{x}) \hat{\psi}_{\mu}(\mathbf{x})$ is the number density (in first and second quantization) and $\hat{\mathbf{j}}$ is the current density of the particle number:

$$(2) \quad \hat{\mathbf{j}}(\mathbf{x}) = \frac{1}{2m} \sum_{i=1}^N [\hat{\mathbf{p}}_i \delta(\mathbf{x} - \hat{\mathbf{x}}_i) + \delta(\mathbf{x} - \hat{\mathbf{x}}_i) \hat{\mathbf{p}}_i]$$

$$(3) \quad \begin{aligned} j_{\ell}(\mathbf{x}) &= \frac{i\hbar}{2m} \sum_{\mu} \left[\frac{\partial \psi_{\mu}^{\dagger}}{\partial x^{\ell}} \psi_{\mu} - \psi_{\mu}^{\dagger} \frac{\partial \psi_{\mu}}{\partial x^{\ell}} \right] \\ &= \frac{i\hbar}{2m} \left(\frac{\partial}{\partial x^{\ell}} - \frac{\partial}{\partial y^{\ell}} \right) \sum_{\mu} \hat{\psi}_{\mu}^{\dagger}(\mathbf{x}) \hat{\psi}_{\mu}(\mathbf{y}) \Big|_{\mathbf{y}=\mathbf{x}} \end{aligned}$$

• *Continuity equation in absence of $\mathbf{A}$.* The meaning of $\mathbf{j}$ as a current for the density is defined by the operator identity

$$(4) \quad [\hat{n}(\mathbf{x}), \hat{H}] = -i\hbar \operatorname{div} \hat{\mathbf{j}}(\mathbf{x})$$

where $\hat{H}$ is the Hamiltonian in absence of vector potential. It implies a continuity equation for the density, with the Heisenberg evolving operators:

$$(5) \quad \frac{\partial}{\partial t} \hat{n}_H(\mathbf{x}, t) = -\operatorname{div} \hat{\mathbf{j}}_H(\mathbf{x}, t)$$

The evaluation of $[\hat{n}(\mathbf{x}), \hat{H}]$ is the actual procedure to obtain the current.

The commutator only involves the kinetic part of $\hat{H}$ and operators of a single particle: $[\delta(\mathbf{y} - \hat{\mathbf{x}}), \hat{\mathbf{p}}^2] = [\delta(\mathbf{y} - \hat{\mathbf{x}}), \hat{\mathbf{p}}] \cdot \hat{\mathbf{p}} + \hat{\mathbf{p}} \cdot [\delta(\mathbf{y} - \hat{\mathbf{x}}), \hat{\mathbf{p}}]$. In the position representation $[\delta(\mathbf{y} - \hat{\mathbf{x}}), \hat{\mathbf{p}}] = i\hbar \nabla_{\mathbf{x}} \delta(\mathbf{y} - \mathbf{x}) = -i\hbar \nabla_{\mathbf{y}} \delta(\mathbf{y} - \mathbf{x})$. Then, for each particle: $[\delta(\mathbf{y} - \hat{\mathbf{x}}), \hat{\mathbf{p}}^2] = -i\hbar \nabla_{\mathbf{y}} [\delta(\mathbf{y} - \hat{\mathbf{x}}) \hat{\mathbf{p}} + \hat{\mathbf{p}} \delta(\mathbf{y} - \hat{\mathbf{x}})]$. The sum on all particles divided by $2m$ gives $\mathbf{j}$. $\square$

- *Continuity equation in presence of $\mathbf{A}$.* Eq.(5) is a continuity equation for the number density with the Hamiltonian $\hat{H}$. With a vector potential the continuity equation defines a new current.

Since $\hat{H}_{\mathbf{A}}$ may depend on time, the Heisenberg time-evolution of the charge density $\hat{\rho}(\mathbf{x}) = q \hat{n}(\mathbf{x})$ is $\hat{\rho}(\mathbf{x}, t) = \hat{U}(t, 0)^\dagger \hat{\rho}(\mathbf{x}) \hat{U}(t, 0)$. With $i\hbar \partial_t \hat{U}(t, 0) = \hat{H}_{\mathbf{A}} \hat{U}(t, 0)$, the equation of motion is:

$$i\hbar \frac{\partial}{\partial t} \hat{\rho}(\mathbf{y}, t) = \hat{U}(t, 0)^\dagger [\hat{\rho}(\mathbf{y}), \hat{H}_{\mathbf{A}}(t)] \hat{U}(t, 0)$$

In the space of a single particle, $\hat{\mathbf{v}} = \frac{1}{m}(\hat{\mathbf{p}} - \frac{q}{c}\mathbf{A})$ are the velocity operators. $[\delta(\mathbf{y} - \hat{\mathbf{x}}), \hat{\mathbf{v}}^2] = \frac{1}{m}[\delta(\mathbf{y} - \hat{\mathbf{x}}), \hat{\mathbf{p}}] \cdot \hat{\mathbf{v}} + \frac{1}{m}\hat{\mathbf{v}} \cdot [\delta(\mathbf{y} - \hat{\mathbf{x}}), \hat{\mathbf{p}}]$. With the results of the previous evaluation we get: $[\delta(\mathbf{y} - \hat{\mathbf{x}}), \hat{\mathbf{v}}^2] = -\frac{i\hbar}{m}\nabla_{\mathbf{y}}[\delta(\mathbf{y} - \hat{\mathbf{x}})\hat{\mathbf{v}} + \hat{\mathbf{v}}\delta(\mathbf{y} - \hat{\mathbf{x}})]$

$$(6) \quad [\hat{\rho}(\mathbf{y}), \hat{H}_{\mathbf{A}}(t)] = -i\hbar \text{div} \hat{\mathbf{J}}(\mathbf{x}, t)$$

with a charged current¹

$$(7) \quad \begin{aligned} \hat{\mathbf{J}}(\mathbf{x}, t) &= \frac{q}{2} \sum_{j=1}^N \delta(\mathbf{y} - \hat{\mathbf{x}}_j) \hat{\mathbf{v}}_j + \hat{\mathbf{v}}_j \delta(\mathbf{y} - \hat{\mathbf{x}}_j) \\ &= q \hat{\mathbf{J}}(\mathbf{x}) - \frac{q^2}{mc} \hat{n}(\mathbf{x}) \mathbf{A}(\mathbf{x}, t) \end{aligned}$$

With the Heisenberg time-evolution of operators being ruled by $\hat{H}_{\mathbf{A}}$, we obtain the continuity equation:

$$(8) \quad \boxed{\frac{\partial}{\partial t} \hat{\rho}_H(\mathbf{x}, t) = -\text{div} \hat{\mathbf{J}}_H(\mathbf{x}, t)}$$

Exercise 1.1. Show that $[v_i, v_j]$ is gauge-invariant. For a uniform and static magnetic field along the z -axis, show that the spectrum of the kinetic Hamiltonian $H = \frac{m}{2}(v_x^2 + v_y^2)$ is discrete (Landau levels).

- *Gauge symmetry.* Consider the unitary operator (written in first and second quantization) with a function Λ :

$$\hat{U}_\Lambda = \exp\left[\frac{iq}{\hbar c} \sum_{j=1}^N \Lambda(\hat{\mathbf{x}}_j, t)\right] = \exp\left[\frac{iq}{\hbar c} \int \hat{n}(\mathbf{x}) \Lambda(\mathbf{x}, t) d\mathbf{x}\right]$$

The action on the Hamiltonian is:

$$\hat{H}'_{\mathbf{A}} = \hat{U}_\Lambda^\dagger \hat{H}_{\mathbf{A}} \hat{U}_\Lambda = \hat{H}_{\mathbf{A} - \nabla \Lambda}$$

It is also $\hat{U}_\Lambda^\dagger \hat{\mathbf{J}} U_\Lambda = \hat{\mathbf{J}} + \frac{q}{mc} \nabla \Lambda$ and $\hat{U}_\Lambda^\dagger \hat{\mathbf{J}} U_\Lambda = \hat{\mathbf{J}} + \frac{q^2}{mc} \nabla \Lambda$.

The action of the unitary operator is compensated by the gauge transformation $\mathbf{A}' = \mathbf{A} + \nabla \Lambda$ of the vector field. Then: $\hat{H}'_{\mathbf{A}'} = \hat{H}_{\mathbf{A}}$ and $\hat{\mathbf{J}}'_{\mathbf{A}'} = \hat{\mathbf{J}}_{\mathbf{A}}$.

¹The two terms in the current are named ‘paramagnetic’ and ‘diamagnetic’.

2. LINEAR RESPONSE

Hereafter we set $q = -e$ (electrons). According to the theory of linear response, once the vector field is turned on at time $t = 0$, a current starts to flow (at equilibrium there is no current, $\langle \mathbf{j} \rangle_{eq} = 0$):

$$\begin{aligned} \langle J_\ell(\mathbf{x}, t) \rangle &= \langle J_\ell(\mathbf{x}, t) \rangle_{eq} + \frac{e}{i\hbar c} \int d\mathbf{x}' dt' \theta(t - t') \langle [-ej_\ell(\mathbf{x}, t), j_m(\mathbf{x}', t')] \rangle_{eq} A_m(\mathbf{x}', t') \\ &= -\frac{e^2}{mc} n(x)_{eq} A_\ell(x) - \frac{e^2}{\hbar c} \int dx' \mathcal{D}_{\ell m}^{ret}(x, x') A_m(x') \end{aligned}$$

with retarded correlator $i\mathcal{D}_{\ell m}^{ret}(x, x') = \theta(t - t') \langle [j_\ell(x), j_m(x')] \rangle$ (repeated space indices are summed). In frequency space:

$$J_\ell(\mathbf{x}, \omega) = -\frac{e^2}{mc} n(\mathbf{x})_{eq} A_\ell(\mathbf{x}, \omega) - \frac{e^2}{\hbar c} \int d\mathbf{x}' \mathcal{D}_{\ell m}^{ret}(\mathbf{x}, \mathbf{x}'; \omega) A_m(\mathbf{x}', \omega)$$

Let $\mathbf{A}$ describe an electric field: $\mathbf{E} = -\frac{1}{c} \frac{\partial \mathbf{A}}{\partial t}$. Then $\mathbf{E}(\mathbf{x}, \omega) = \frac{i\omega}{c} \mathbf{A}(\mathbf{x}, \omega)$ and

$$(9) \quad J_\ell(\mathbf{x}, \omega) = \int d\mathbf{x}' \sigma_{\ell m}(\mathbf{x}, \mathbf{x}'; \omega) E_m(\mathbf{x}', \omega)$$

with conductivity tensor

$$\sigma_{\ell m}(\mathbf{x}, \mathbf{x}'; \omega) = -\frac{e^2}{im\omega} n(\mathbf{x}) \delta(\mathbf{x} - \mathbf{x}') \delta_{\ell m} - \frac{e^2}{i\hbar\omega} \mathcal{D}_{\ell m}^{ret}(\mathbf{x}, \mathbf{x}', \omega)$$

For a homogeneous system the linear relation is

$$(10) \quad \boxed{J_\ell(\mathbf{k}, \omega) = \sigma_{\ell m}(\mathbf{k}, \omega) E_m(\mathbf{k}, \omega)}$$

$$\sigma_{\ell m}(\mathbf{k}; \omega) = -\frac{e^2}{im\omega} n \delta_{\ell m} - \frac{e^2}{i\hbar\omega} \mathcal{D}_{\ell m}^{ret}(\mathbf{k}, \omega)$$

A cancellation of imaginary terms must occur, to give the conductivity tensor that appears in Ohm's law. Then

$$(11) \quad \boxed{\sigma_{\ell m}(\mathbf{k}; \omega) = -\text{Im} \frac{e^2}{\hbar\omega} \mathcal{D}_{\ell m}^{ret}(\mathbf{k}; \omega)}$$

For a uniform and constant electric field the limits $k \rightarrow 0$ and $\omega \rightarrow 0$ are taken. The singularity in $\omega = 0$ must be compensated by the numerator.

3. THE CURRENT-CURRENT CORRELATOR

An interesting model for a microscopic deduction of the conductivity tensor consists of free electrons that scatter on fixed random impurities, with short range potential.

The conductivity tensor results from the analytic continuation of the imaginary time-ordered correlator

$$(12) \quad \begin{aligned} -\mathcal{D}_{\ell m}(\mathbf{x}, \tau; \mathbf{x}', \tau') &= \langle \mathcal{T} \delta j_\ell(\mathbf{x}, \tau) \delta j_m(\mathbf{x}', \tau') \rangle_{eq} \\ &= \left(\frac{i\hbar}{2m} \right)^2 \sum_{\mu\nu} \left[\frac{\partial}{\partial x_\ell} - \frac{\partial}{\partial y_\ell} \right] \left[\frac{\partial}{\partial x'_m} - \frac{\partial}{\partial y'_m} \right] \langle \mathcal{T} \psi_\mu^\dagger(x) \psi_\mu(y) \psi_\nu^\dagger(x') \psi_\nu(y') \rangle \end{aligned}$$

where, in the end, $y = x$ and $y' = x'$, and only the connected parts are taken.

For electrons that only interact with the impurities, Wick's theorem applies, and the connected correlator factors into a pair of propagators. After the derivatives,

and setting $x = y$ and $x' = y'$, one pair gives two disconnected bubble diagrams and is discarded. The other pair gives a single diagram, whose expression depends on the positions of the scatterers.

To avoid such unmanageable dependence, one considers the problem at a scale much larger than the average distance of the scatterers, where it is meaningful to average the correlator in the random positions of the scatterers. In doing so, it is not true that the average of the correlator is the product of two averaged Green functions. There are correlations among the two particles, as they may interact with the same impurities. These correlations appear as vertex corrections².

If we neglect such correlations, we are in a Hartree Fock approximation:

$$\overline{\langle \mathcal{T} \psi_\mu^\dagger(x) \psi_\mu(y) \psi_\nu^\dagger(x') \psi_\nu(y') \rangle} \approx -\mathcal{G}_{\mu\nu}(y, x') \mathcal{G}_{\nu\mu}(y', x)$$

where the Green functions are averaged. The average makes them translation-invariant. We assume that $\mathcal{G}_{\mu\nu} = \delta_{\mu\nu} \mathcal{G}$:

$$\begin{aligned} \mathcal{D}_{\ell m}(x, x') &= 2 \left(\frac{i\hbar}{2m} \right)^2 \left(\frac{\partial}{\partial x_\ell} - \frac{\partial}{\partial y_\ell} \right) \left(\frac{\partial}{\partial x'_m} - \frac{\partial}{\partial y'_m} \right) \mathcal{G}(y, x') \mathcal{G}(y', x) \Big|_{x=y, x'=y'} \\ &= 2i^2 \left(\frac{i\hbar}{2m} \right)^2 \int \frac{d\mathbf{k} d\mathbf{q}}{(2\pi)^6} (k_\ell + q_\ell)(q_m + k_m) \mathcal{G}(\mathbf{k}, \tau - \tau') \mathcal{G}(\mathbf{q}, \tau' - \tau) e^{i(\mathbf{k}-\mathbf{q}) \cdot (\mathbf{x}-\mathbf{x}')} \\ \mathcal{D}_{\ell m}(\mathbf{k}, i\nu) &= 2 \left(\frac{\hbar}{2m} \right)^2 \frac{1}{\hbar\beta} \sum_{i\omega} \int \frac{d\mathbf{q}}{(2\pi)^3} (k_\ell + 2q_\ell)(k_m + 2q_m) \mathcal{G}(\mathbf{k} + \mathbf{q}, i\omega + i\nu) \mathcal{G}(\mathbf{q}, i\omega) \end{aligned}$$

Let us insert the spectral representation of the averaged propagator:

$$\mathcal{G}(\mathbf{k}, i\omega) = \int d\omega' \frac{A(\mathbf{k}, \omega')}{i\omega - \omega'}$$

The Matsubara sum is done and gives:

$$\mathcal{D}_{\ell m}(\mathbf{k}, i\nu) = -\frac{\hbar^2}{2m^2} \int \frac{d\mathbf{q}}{(2\pi)^3} d\omega' d\omega'' (k_\ell + 2q_\ell)(k_m + 2q_m) A(\mathbf{k} + \mathbf{q}, \omega') A(\mathbf{q}, \omega'') \frac{n(\omega') - n(\omega'')}{i\nu - (\omega' - \omega'')}$$

This expression has the form of a Lehmann representation of the correlator. The retarded function is obtained by the replacement $i\nu \rightarrow \nu + i\eta$.

$$\begin{aligned} \mathcal{D}_{\ell m}^{ret}(\mathbf{k}, \nu) &= -\frac{\hbar^2}{2m^2} \int \frac{d\mathbf{q}}{(2\pi)^3} (k_\ell + 2q_\ell)(k_m + 2q_m) \\ &\quad \int d\omega' d\omega'' A(\mathbf{k} + \mathbf{q}, \omega') A(\mathbf{q}, \omega'') \frac{n(\omega') - n(\omega'')}{\nu - (\omega' - \omega'') + i\eta} \end{aligned}$$

The imaginary part is obtained via the Plemelj-Sokhotski formula. The delta function is used to perform the integral in ω' :

$$\begin{aligned} \text{Im} \mathcal{D}_{\ell m}^{ret}(\mathbf{k}, \nu) &= \frac{\pi \hbar^2}{2m^2} \int \frac{d\mathbf{q}}{(2\pi)^3} (k_\ell + 2q_\ell)(k_m + 2q_m) \\ &\quad \int d\omega A(\mathbf{k} + \mathbf{q}, \omega + \nu) A(\mathbf{q}, \omega) [n(\omega + \nu) - n(\omega)] \end{aligned}$$

The ‘static’ and uniform limit of conductivity exists:

$$\sigma_{\ell m}(0) = -\frac{e^2}{\hbar} \lim_{\nu \rightarrow 0} \frac{1}{\nu} \text{Im} \mathcal{D}_{\ell m}^{ret}(0, \nu) = -\frac{e^2}{\hbar} \frac{4\pi \hbar^2}{2m^2} \int \frac{d\mathbf{q}}{(2\pi)^3} q_\ell q_m \int d\omega A^2(\mathbf{q}, \omega) \frac{dn(\omega)}{d\omega}$$

²see Ch.8 in Mahan, Many particle physics, 3rd Edition, Kluwer Academics, 2000.

If the system is isotropic, the integral is proportional to $\delta_{\ell m}$, then:

$$(13) \quad \sigma(0) = \frac{4\pi e^2}{3\hbar m} \int \frac{d\mathbf{q}}{(2\pi)^3} \frac{\hbar^2 q^2}{2m} \int_{-\infty}^{+\infty} d\omega A^2(q, \omega) \left(-\frac{dn(\omega)}{d\omega} \right)$$

This is eq. 8.49 in Mahan's book (3rd ed.). For $T \rightarrow 0$ it is $n(\omega) = \theta(\frac{\mu}{\hbar} - \omega)$, then

$$(14) \quad \sigma(0) = \frac{4\pi e^2}{3m\hbar} \int \frac{d\mathbf{q}}{(2\pi)^3} \epsilon_q A^2(q, \frac{\mu}{\hbar}) = \frac{4\pi e^2}{3m\hbar} \int_0^\infty d\epsilon \rho(\epsilon) \epsilon A^2(q, \frac{\mu}{\hbar})$$

Let us use the following form of spectral function, which is explained by the theory of electrons in the random environment

$$(15) \quad A(q, \omega) = \frac{1}{2\pi\tau} \frac{1}{(\omega - \frac{\epsilon_q}{\hbar})^2 + \frac{1}{(2\tau)^2}}$$

The integral can be extended to $-\infty$ as the function is evaluated at $\hbar\omega = \mu$ and is peaked around this value. The density, having slow variation near $\epsilon = \mu$, is factored out. The integral becomes:

$$\frac{1}{4\pi^2\tau^2} \int_{-\infty}^{+\infty} d\epsilon \frac{\epsilon}{[(\frac{\mu-\epsilon}{\hbar})^2 + \frac{1}{(2\tau)^2}]^2} = \frac{\hbar\tau}{\pi}$$

With $\mu\rho(\mu) = \frac{3}{4}n$, a Drude-like formula for the d.c. (direct current) conductivity is obtained:

$$(16) \quad \boxed{\sigma_{d.c.}(0) = \frac{e^2 n}{m} \tau}$$

Here τ is the life-time provided by the 1-particle Green function, and it is evaluated in the next section. The omitted vertex corrections provide a different relaxation life-time.

4. A MODEL WITH RANDOM SCATTERERS

A box of volume V contains N_I impurities randomly distributed, with uniform probability, at positions $\mathbf{R}_j$. The potential energy felt by a particle is the sum of the impurity potentials:

$$V(\mathbf{x}) = \sum_{j=1}^{N_I} v(\mathbf{x} - \mathbf{R}_j) = \frac{1}{V} \sum_{\mathbf{k}} \tilde{v}(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{x}} \sum_{j=1}^{N_I} e^{-i\mathbf{k}\cdot\mathbf{R}_j}$$

The range of the potential v is assumed to be much shorter than the mean separation of the scatterers $n_I^{-1/3}$, where $n_I = N_I/V$.

The one-particle thermal Green function is expanded in Born series

$$g(1, 2) = g^0(1, 2) + \frac{1}{\hbar} g^0(1, 3) V(3) g^0(3, 2) + \frac{1}{\hbar^2} g^0(1, 3) V(3) g^0(1, 4) V(4) g^0(4, 2) + \dots$$

On a scale much larger than the separation of the scatterers, the particle loses memory of the positions of the scatterers, and one may replace g with an average on the random positions of the impurities. This requires the evaluation of averages

$$\overline{V(\mathbf{x}_1) \dots V(\mathbf{x}_k)} = \int \frac{d\mathbf{R}_1 \dots d\mathbf{R}_{N_I}}{V^{N_I}} V(\mathbf{x}_1) \dots V(\mathbf{x}_k)$$

In the limit of large V with finite density n_I :

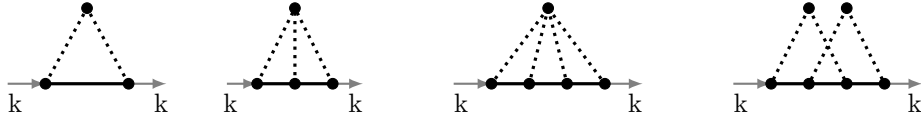
$$\begin{aligned}\overline{V(\mathbf{x})} &= n_I \tilde{v}(0); \\ \overline{V(\mathbf{x}_1)V(\mathbf{x}_2)} &= \frac{n_I}{V} \sum_{\mathbf{k}} \tilde{v}(\mathbf{k})\tilde{v}(-\mathbf{k})e^{i\mathbf{k}\cdot(\mathbf{x}_1-\mathbf{x}_2)} + [n_I \tilde{v}(0)]^2 \\ \overline{V(\mathbf{x}_1)V(\mathbf{x}_2)V(\mathbf{x}_3)} &= \frac{n_I}{V^2} \sum_{\mathbf{k}_1 \mathbf{k}_2} \tilde{v}(\mathbf{k}_1)\tilde{v}(\mathbf{k}_2)\tilde{v}(-\mathbf{k}_1 - \mathbf{k}_2)e^{i\mathbf{k}_1\cdot(\mathbf{x}_1-\mathbf{x}_3)+i\mathbf{k}_2\cdot(\mathbf{x}_2-\mathbf{x}_3)} \\ &\quad + \left(\overline{V(\mathbf{x}_1)V(\mathbf{x}_2)} + \overline{V(\mathbf{x}_2)V(\mathbf{x}_3)} + \overline{V(\mathbf{x}_1)V(\mathbf{x}_3)} \right) [n_I \tilde{v}(0)] + [n_I \tilde{v}(0)]^3\end{aligned}$$

The factors $n_I \tilde{v}(0)$ may be removed by a Hartree resummation that only shifts the energy:

$$g_H(k, i\omega) = \frac{1}{i\omega - \frac{1}{\hbar}(\epsilon_k - \mu + n_I \tilde{v}(0))}$$

We continue to use the symbol g for the Hartree function. The averaged Born series becomes: $\mathcal{G}(1, 2) = g_H(1, 2) + g_H(1, 3)[\frac{1}{\hbar^2} \overline{V(3)}g_H(1, 4)\overline{V(4)}]g_H(4, 2) + \dots$. Each term is now translation invariant. In $k = (\mathbf{k}, i\omega_n)$ space the first terms of the Born expansion are:

$$\begin{aligned}\mathcal{G}(k) &= g(k) + g(k)\Sigma^{(2)}(k)g(k) + g(k)\Sigma^{(3)}(k)g(k) + g(k)\Sigma^{(4)}(k)g(k) \\ &\quad + g(k)\Sigma^{(2)}(k)g(k)\Sigma^{(2)}(k)g(k) + g(k)\Sigma^{(4cr)}(k)g(k) + \dots\end{aligned}$$



The self-energy terms $\Sigma^{(2)}(k, i\omega_n)$, $\Sigma^{(3)}(k, i\omega_n)$, $\Sigma^{(4)}(k, i\omega_n)$ are order n_I . The crossed term is order n_I^2 and is neglected.

Let's compute the first crossed diagram to show that it is of order n_I^2 :

$$\begin{aligned}\Sigma^{(4,cr)}(\mathbf{x}_1, \mathbf{x}_4, i\omega_n) &= \frac{1}{\hbar^4} \iint d\mathbf{x}_2 d\mathbf{x}_3 \overline{V(\mathbf{x}_1)}g(1, 2)\overline{V(\mathbf{x}_3)}g(2, 3)\overline{V(\mathbf{x}_2)}g(3, 4)\overline{V(\mathbf{x}_4)} \\ &= \frac{n_I^2}{\hbar^2 V^2} \sum_{\mathbf{k}, \mathbf{k}'} |\tilde{v}(\mathbf{k})|^2 |\tilde{v}(\mathbf{k}')|^2 \iint d\mathbf{x}_2 d\mathbf{x}_3 e^{i\mathbf{k}\cdot(\mathbf{x}_1-\mathbf{x}_3)} e^{i\mathbf{k}'\cdot(\mathbf{x}_2-\mathbf{x}_4)} g(1, 2)g(2, 3)g(3, 4) \\ &= \frac{n_I^2}{\hbar^2 V^3} \sum_{\mathbf{k}, \mathbf{k}', \mathbf{q}} |\tilde{v}(\mathbf{k})|^2 |\tilde{v}(\mathbf{k}')|^2 g(\mathbf{q} + \mathbf{k}', i\omega_n)g(\mathbf{q}, i\omega_n)g(\mathbf{q} + \mathbf{k}, i\omega_n) e^{i(\mathbf{q}+\mathbf{k}+\mathbf{k}')\cdot(\mathbf{x}_1-\mathbf{x}_4)}. \\ \Sigma^{(4,cr)}(\mathbf{p}, i\omega_n) &= \frac{n_I^2}{V^2} \sum_{\mathbf{k}, \mathbf{k}'} |\tilde{v}(\mathbf{k})|^2 |\tilde{v}(\mathbf{k}')|^2 g(\mathbf{p} - \mathbf{k}, i\omega_n)g(\mathbf{p} - \mathbf{k} - \mathbf{k}', i\omega_n)g(\mathbf{p} - \mathbf{k}', i\omega_n)\end{aligned}$$

1) A non-trivial partial resummation, valid for low density n_I of scatterers, is done with the self-energy $\Sigma^{(2)}(1, 2) = \frac{1}{\hbar^2} \overline{V(1)}g(1, 2)\overline{V(2)}$. In momentum space:

$$\Sigma(\mathbf{k}, i\omega_n) = \frac{n_I}{\hbar^2} \int \frac{d\mathbf{q}}{(2\pi)^3} \frac{|\tilde{v}(\mathbf{q} - \mathbf{k})|^2}{i\omega - \frac{1}{\hbar}(\epsilon_q - \mu)}$$

The retarded function is obtained with $i\omega_n \rightarrow \omega + i\eta$. We are interested in the imaginary part (lifetime). The energy is measured with respect to the chemical

potential. We take $\omega = 0$.

$$\frac{1}{2\tau_k} = -\text{Im}\Sigma^R(k, 0) = \frac{\pi n_I}{\hbar} \int \frac{d\mathbf{q}}{(2\pi)^3} |\tilde{v}(\mathbf{q} - \mathbf{k})|^2 \delta(\epsilon_q - \mu)$$

In this approximation, the retarded Green function has the form

$$\mathcal{G}^R(\mathbf{k}, \omega) = \frac{1}{\omega - \frac{1}{\hbar}(\tilde{\epsilon}_k - \mu) + i\frac{1}{2\tau_k}}$$

with a new dispersion law $\tilde{\epsilon}(k)$. The retarded function gives the spectral function:

$$A(k, \omega) = -\frac{1}{\pi} \text{Im} \mathcal{G}^{ret}(k, \omega) = \frac{1}{2\pi\tau_k} \frac{1}{(\omega - \frac{\tilde{\epsilon}_k - \mu}{\hbar})^2 + \frac{1}{4\tau_k^2}}$$

2) With the following self-energy, the averages of order n_I are summed (nested diagrams are not included):

$$\begin{aligned} \Sigma^*(1, 2) &= \frac{n_I}{\hbar} \tilde{v}(0) \delta(1, 2) + \frac{1}{\hbar^2} \overline{V(1)g(1, 2)V(2)} + \frac{1}{\hbar^3} \overline{V(1)g(1, 3)V(3)g(3, 2)V(2)} \\ &+ \frac{1}{\hbar^4} \overline{V(1)g(1, 3)V(3)g(3, 4)V(4)g(4, 2)V(2)} + \dots \end{aligned}$$

In momentum space it is:

$$\begin{aligned} \Sigma^*(\mathbf{k}, i\omega) &= \frac{n_I}{\hbar} \tilde{v}(0) + \frac{n_I}{\hbar^2} \int \frac{d\mathbf{q}}{(2\pi)^3} \tilde{v}(\mathbf{q}) g(\mathbf{k} + \mathbf{q}, i\omega) \tilde{v}(-\mathbf{q}) \\ &+ \frac{n_I}{\hbar^3} \int \frac{d\mathbf{q}_1 d\mathbf{q}_2}{(2\pi)^6} \tilde{v}(\mathbf{q}_1) g(\mathbf{k} + \mathbf{q}_1, i\omega) \tilde{v}(\mathbf{q}_2) g(\mathbf{k} + \mathbf{q}_1 + \mathbf{q}_2, i\omega) \tilde{v}(-\mathbf{q}_1 - \mathbf{q}_2) + \dots \end{aligned}$$

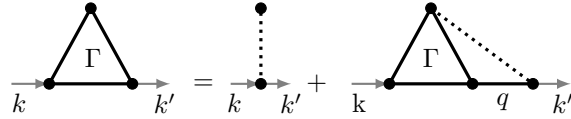
The sum can be done by introducing an auxiliary function where momentum conservation is violated:

$$\begin{aligned} \Gamma(\mathbf{k}, \mathbf{k}', i\omega) &= \frac{1}{\hbar} \tilde{v}(\mathbf{k}' - \mathbf{k}) + \frac{1}{\hbar^2} \int \frac{d\mathbf{q}}{(2\pi)^3} \tilde{v}(\mathbf{q}) g(\mathbf{k} + \mathbf{q}, i\omega) \tilde{v}(\mathbf{k}' - \mathbf{k} - \mathbf{q}) \\ &+ \frac{1}{\hbar^3} \int \frac{d\mathbf{q}_1 d\mathbf{q}_2}{(2\pi)^6} \tilde{v}(\mathbf{q}_1) g(\mathbf{k} + \mathbf{q}_1, i\omega) \tilde{v}(\mathbf{q}_2) g(\mathbf{k} + \mathbf{q}_1 + \mathbf{q}_2, i\omega) \tilde{v}(\mathbf{k}' - \mathbf{k} - \mathbf{q}_1 - \mathbf{q}_2) + \dots \end{aligned}$$

It is $\Sigma^*(\mathbf{k}, i\omega) = n_I \Gamma(\mathbf{k}, \mathbf{k}, i\omega)$.

The function Γ solves a Dyson equation (see figure):

$$\Gamma(\mathbf{k}, \mathbf{k}', i\omega) = \frac{1}{\hbar} \tilde{v}(\mathbf{k}' - \mathbf{k}) + \frac{1}{\hbar} \int \frac{d\mathbf{q}}{(2\pi)^3} \Gamma(\mathbf{k}, \mathbf{q}, i\omega) g(\mathbf{q}, i\omega) \tilde{v}(\mathbf{k}' - \mathbf{q})$$



The Dyson equation for $\Gamma(k, k', i\omega_n)$.

The Dyson equation of the T -matrix is: $\hat{T}(E) = \hat{v} + \hat{T}(E) \frac{1}{E - \hbar + i\eta} \hat{v}$. Take the matrix elements with $\langle \mathbf{k} | \hat{v} | \mathbf{k}' \rangle = \int d\mathbf{x} v(\mathbf{x}) e^{i(\mathbf{k}' - \mathbf{k}) \cdot \mathbf{x}} / (2\pi)^3 = \tilde{v}(\mathbf{k}' - \mathbf{k}) / (2\pi)^3$:

$$(2\pi)^3 \langle \mathbf{k} | T(E) | \mathbf{k}' \rangle = \tilde{v}(\mathbf{k}' - \mathbf{k}) + \int d\mathbf{q} \langle \mathbf{k} | T(E) | \mathbf{q} \rangle \frac{1}{E - \epsilon_q + i\eta} \tilde{v}(\mathbf{k}' - \mathbf{q})$$

with $i\omega = \frac{E}{\hbar}$ the two equations identify with $\hbar\Gamma^{ret}(\mathbf{k}, \mathbf{k}', \frac{1}{\hbar}E) = (2\pi)^3 \langle \mathbf{k} | \hat{T}(E) | \mathbf{k}' \rangle$. Then we obtain eq. 4.114 in Mahan's book:

$$\begin{aligned} \text{Im } \Sigma^{ret}(\mathbf{k}, \frac{E}{\hbar}) &= \frac{n_I}{\hbar} (2\pi)^3 \text{Im} \langle \mathbf{k} | \hat{T}(E) | \mathbf{k} \rangle \\ &= \frac{n_I}{\hbar} (2\pi)^3 \frac{-\hbar^2 k}{16\pi^3 m} \sigma(E) \\ (17) \quad &= -\frac{1}{2} n_I v(k) \sigma(k) \end{aligned}$$

$v(E) = \hbar k/m$ is the velocity, $\sigma(k)$ is the total cross section for scattering on a single impurity at momentum k . It follows that the life-time is the mean time between two scattering events:

$$(18) \quad \frac{1}{\tau(k)} = n_I v(k) \sigma(k)$$

The inclusion of vertex corrections in the evaluation of $\langle T_{jl}(x) j_m(y) \rangle$ modifies the characteristic time by an angular term in the integral that accounts for the fact that scattering at small angles affects transport less than scattering at large angles. See eq.(22).

5. THE BOLTZMANN EQUATION (1872)

Let $f(\mathbf{x}, \mathbf{p}, t) d\mathbf{x} d\mathbf{p}$ be the number of particles at time t in the volume $d\mathbf{x} d\mathbf{p}$ of phase space, centred in $(\mathbf{x}, \mathbf{p})$. The number and the current densities are

$$\int d\mathbf{p} f(\mathbf{x}, \mathbf{p}, t), \quad \int d\mathbf{p} f(\mathbf{x}, \mathbf{p}, t) \frac{\mathbf{p}}{m}$$

A kinetic equation describes the time evolution of the phase-space density of particles: there is a time variation due to the Hamiltonian flow, and a variation, on a short time scale, due to collisions (see K. Huang, Statistical Mechanics, J. Wiley):

$$(19) \quad \frac{\partial f}{\partial t} + \frac{\partial f}{\partial \mathbf{x}} \cdot \frac{\mathbf{p}}{m} + \frac{\partial f}{\partial \mathbf{p}} \mathbf{F} = \left(\frac{\partial f}{\partial t} \right)_{\text{coll}}$$

$\mathbf{F}$ is the local external force acting on particles, the collision term involves joint two-particle distributions before and after a two-body collision, and a scattering probability. In the Boltzmann equation $f_2(\mathbf{x}_1, \mathbf{p}_1; \mathbf{x}_2, \mathbf{p}_2; t) = f(\mathbf{x}_1, \mathbf{p}_1; t) f(\mathbf{x}_2, \mathbf{p}_2; t)$ (hypothesis of molecular chaos). As such, it is a truncation of the BBGKY (Bogoliubov, Born, Green, Kirkwood and Yvonne, around 1940) hierarchy of equations for the distribution functions of many particles.

$$\left(\frac{\partial f}{\partial t} \right)_{\text{coll}} = \int d\mathbf{q} \pi(\mathbf{p}, \mathbf{q} \rightarrow \mathbf{p}', \mathbf{q}') [f(\mathbf{x}, \mathbf{p}', t) f(\mathbf{x}, \mathbf{q}', t) - f(\mathbf{x}, \mathbf{p}, t) f(\mathbf{x}, \mathbf{q}, t)]$$

At $(\mathbf{x}, t)$ an *elastic* collision takes place, with $\mathbf{p}, \mathbf{q} \leftrightarrow \mathbf{p}', \mathbf{q}'$. Then $\mathbf{p} + \mathbf{q} = \mathbf{p}' + \mathbf{q}'$ and $p^2 + q^2 = p'^2 + q'^2$.

5.1. The H theorem. For a gas of particles, Boltzmann showed that f tends to the Maxwell-Boltzmann thermal distribution, and proved the H -theorem. The theorem states that $H(t) = \int d\mathbf{x} d\mathbf{p} f(\mathbf{x}, \mathbf{p}, t) \log f(\mathbf{x}, \mathbf{p}, t)$ decreases in time.

$$\begin{aligned} \frac{dH}{dt} &= \int d\mathbf{x} d\mathbf{p} \frac{\partial f}{\partial t} [1 + \log f] = \int d\mathbf{x} d\mathbf{p} \left(\frac{\partial f}{\partial t} \right)_{\text{coll}} [1 + \log f] \\ &= \int d\mathbf{x} d\mathbf{p} d\mathbf{q} \pi(\mathbf{p}, \mathbf{q} \rightarrow \mathbf{p}', \mathbf{q}') [f(\mathbf{x}, \mathbf{p}', t) f(\mathbf{x}, \mathbf{q}', t) - f(\mathbf{x}, \mathbf{p}, t) f(\mathbf{x}, \mathbf{q}, t)] [1 + \log f(\mathbf{x}, \mathbf{p}, t)] \end{aligned}$$

The Hamiltonian flow contains gradients, which give boundary terms that vanish. Now interchange particles with momenta $\mathbf{p}$ and $\mathbf{q}$ and sum:

$$\begin{aligned} \frac{dH}{dt} = \int d\mathbf{x} d\mathbf{p} d\mathbf{q} \pi(\mathbf{p}, \mathbf{q} \rightarrow \mathbf{p}', \mathbf{q}') [f(\mathbf{x}, \mathbf{p}', t) f(\mathbf{x}, \mathbf{q}', t) - f(\mathbf{x}, \mathbf{p}, t) f(\mathbf{x}, \mathbf{q}, t)] \\ [1 + \frac{1}{2} \log f(\mathbf{x}, \mathbf{p}, t) f(\mathbf{x}, \mathbf{q}, t)] \end{aligned}$$

Finally add the expression with initial and final states exchanged, and use $d\mathbf{p} d\mathbf{q} = d\mathbf{p}' d\mathbf{q}'$. The rate π is unchanged:

$$\begin{aligned} \frac{dH}{dt} = \frac{1}{4} \int d\mathbf{x} d\mathbf{p} d\mathbf{q} \pi(\mathbf{p}, \mathbf{q} \rightarrow \mathbf{p}', \mathbf{q}') [f(\mathbf{x}, \mathbf{p}', t) f(\mathbf{x}, \mathbf{q}', t) - f(\mathbf{x}, \mathbf{p}, t) f(\mathbf{x}, \mathbf{q}, t)] \\ \log \frac{f(\mathbf{x}, \mathbf{p}, t) f(\mathbf{x}, \mathbf{q}, t)}{f(\mathbf{x}, \mathbf{p}', t) f(\mathbf{x}, \mathbf{q}', t)} \end{aligned}$$

By the inequality $(y - x)(\log x - \log y) \leq 0$ we conclude that:

$$(20) \quad \frac{dH(t)}{dt} \leq 0$$

The entropy is defined as $S = -k_B H$. The function H decreases and becomes stationary at equilibrium if, everywhere: $\log f(\mathbf{p}') + \log f(\mathbf{q}') = \log f(\mathbf{p}) + \log f(\mathbf{q})$. For a homogeneous system, since momentum and kinetic energy are conserved, it must be:

$$\log f(\mathbf{p}) = a + \mathbf{b} \cdot \mathbf{p} + c p^2$$

This gives the Maxwell-Boltzmann distribution.

Chapman and Enskog (1917), by exploiting the symmetries of the scattering term, gave a microscopic derivation of the hydrodynamical description of matter.

5.2. Conductivity. For the problem of transport, in presence of a uniform and static electric field, we seek a stationary and homogeneous solution, in the relaxation-time approximation:

$$(21) \quad \frac{1}{\hbar} \frac{\partial f(\mathbf{k})}{\partial \mathbf{k}} (-e \mathbf{E}) = -\frac{f(\mathbf{k}) - f_0(\mathbf{k})}{\tau_t(\mathbf{k})}$$

where we replaced $\mathbf{p}$ with $\hbar \mathbf{k}$ and it is $f_0(\mathbf{k}) = 2[e^{\beta(\epsilon_{\mathbf{k}} - \mu)} + 1]^{-1}$ (the factor 2 is due to spin). τ_t is a relaxation time related to transport.

To linear order:

$$f(\mathbf{k}) = f_0(k) + \frac{e \tau_t(\mathbf{k})}{\hbar} \frac{\partial f_0}{\partial \epsilon} \frac{\hbar^2}{m} \mathbf{k} \cdot \mathbf{E}$$

With $\mathbf{v} = \hbar \mathbf{k}/m$, the charged current density is

$$\mathbf{J} = -e \int \frac{d\mathbf{k}}{(2\pi)^3} f(\mathbf{k}) \mathbf{v} = -e^2 \int \frac{d\mathbf{k}}{(2\pi)^3} \tau_t(\mathbf{k}) \frac{\partial f_0}{\partial \epsilon_k} \mathbf{v} (\mathbf{v} \cdot \mathbf{E})$$

If the system is isotropic, we replace $v_i v_j$ with $\frac{1}{3} v^2 \delta_{ij}$ and $v^2 = \frac{2}{m} \epsilon$. We read $J = \sigma E$ with

$$\sigma = -\frac{2e^2}{3m} \int \frac{d\mathbf{k}}{(2\pi)^3} \frac{\partial f_0}{\partial \epsilon_k} \epsilon_k \tau_t(k) = -\frac{2e^2}{3m} \int d\epsilon \rho(\epsilon) \frac{\partial f_0}{\partial \epsilon} \epsilon \tau_t(\epsilon)$$

In the limit of low T , $f_0 = 2\theta(\epsilon_F - \epsilon)$. The formula by Drude is obtained (with $\rho(\epsilon_F) \epsilon_F = \frac{3}{4} n$):

$$\sigma = \frac{4e^2}{3m} \rho(\epsilon_F) \epsilon_F \tau_t(\epsilon_F) = \frac{e^2 n \tau_t(\epsilon_F)}{m}$$

Note: the relaxation time τ_t is for electrons at the Fermi surface, but the density is that of all conduction electrons (not only those near the Fermi surface). The relaxation time is not the same as the time interval among scattering events (as obtained from the self-energy).

The transport relaxation time is evaluated (Mahan, eq.8.25) by writing the collision term explicitly. In the collision with an impurity, momentum is changed from $\mathbf{k}$ to $\mathbf{k}'$ and back, of same modulus. The number of scatterings $\mathbf{k} \rightarrow \mathbf{k}'$ per unit time and unit volume is

$$2\pi n_I \int \frac{d\mathbf{k}'}{(2\pi)^3} \delta(\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}'}) |T_{\mathbf{k}\mathbf{k}'}|^2 f(\mathbf{k}) [1 - f(\mathbf{k}')]]$$

the opposite process has rate $2\pi n_I \int \frac{d\mathbf{k}'}{(2\pi)^3} \delta(\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}'}) |T_{\mathbf{k}'\mathbf{k}}|^2 f(\mathbf{k}') [1 - f(\mathbf{k})]$. The difference gives the collisional variation (T-matrix is Hermitian):

$$\begin{aligned} \left(\frac{df}{dt} \right)_{coll} &= 2\pi n_I \int \frac{d\mathbf{k}'}{(2\pi)^3} \delta(\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}'}) |T_{\mathbf{k}'\mathbf{k}}|^2 [f(\mathbf{k}') - f(\mathbf{k})] \\ &= 2\pi n_I \frac{e\hbar\tau_t(k)}{m^2} \frac{\partial f_0}{\partial \epsilon} \int \frac{d\mathbf{k}'}{(2\pi)^3} \delta(\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}'}) |T_{\mathbf{k}'\mathbf{k}}|^2 (\mathbf{k}' - \mathbf{k}) \cdot \mathbf{E} \end{aligned}$$

The T matrix depends on the angle θ' between the vectors $\mathbf{k}$ and $\mathbf{k}'$. In polar coordinates, with $\mathbf{k}$ along z -axis and $\mathbf{E}$ in the xz -plane, it is: $\mathbf{k}' = k(\sin \theta' \cos \varphi', \sin \theta' \sin \varphi', \cos \theta')$ and $\mathbf{E} = E(\sin \theta, 0, \cos \theta)$. Therefore:

$$(\mathbf{k}' - \mathbf{k}) \cdot \mathbf{E} = kE(\sin \theta' \cos \varphi' \sin \theta + \cos \theta' \cos \theta - \cos \theta)$$

The angular integral in φ' cancels the first term, then:

$$\begin{aligned} \left(\frac{df}{dt} \right)_{coll} &= -2\pi n_I \frac{e\hbar\tau_t(k)}{m^2} \frac{\partial f_0}{\partial \epsilon} \int \frac{d\mathbf{k}'}{(2\pi)^3} \delta(\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}'}) |T_{\mathbf{k}'\mathbf{k}}|^2 (1 - \cos \theta') \mathbf{k} \cdot \mathbf{E} \\ &= -2\pi n_I [f(\mathbf{k}) - f_0(k)] \int \frac{d\mathbf{k}'}{(2\pi)^3} \delta(\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}'}) |T_{\mathbf{k}'\mathbf{k}}|^2 (1 - \cos \theta') \end{aligned}$$

A cancellation occurs with the left-hand side and what remains is:

$$(22) \quad \frac{1}{\tau_t(k)} = 2\pi n_I \int \frac{d\mathbf{k}'}{(2\pi)^3} \delta(\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}'}) |\langle \mathbf{k} | \hat{T}(\epsilon) | \mathbf{k}' \rangle|^2 \left(1 - \frac{\mathbf{k} \cdot \mathbf{k}'}{k^2} \right)$$

The relaxation time with the self-energy is the same integral, without the angular factor. The latter takes into account the geometry of scattering.

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