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CONDUCTIVITY TENSOR

1. CURRENTS

In first quantisation, the Hamiltonian operator for N identical particles with charge q, in an e.m. field with vector potential $\mathbf{A}(\mathbf{x},t)$ is

$$H = \sum_{i=1}^{N} \frac{m}{2}\hat{\mathbf{v}}_i^2(t) + U(\hat{\mathbf{x}}_1,...,\hat{\mathbf{x}}_n), \qquad \hat{\mathbf{v}}_i = \frac{1}{m}\hat{\mathbf{p}}_i - \frac{q}{mc}\mathbf{A}(\hat{\mathbf{x}}_i,t) \tag{1}$$

where $\mathbf{v}$ is the velocity operator. The charge density of particles is $\rho(\mathbf{x}) = q\,n(\mathbf{x})$, where $n(\mathbf{x}) = \sum_{i=1}^{N}\delta(\mathbf{x}-\hat{\mathbf{x}}_i)$ is the (number) density. It evolves in time as $\rho_H(\mathbf{x},t) = U(t,0)^\dagger\rho(\mathbf{x})U(t,0)$, where the propagator solves $i\hbar\partial_t U(t,0) = H(t)U(t,0)$. Then

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

The commutator only involves the kinetic part, and operators of the same particle. In the space of a single particle: $[\delta(\mathbf{y}-\hat{\mathbf{x}}),\hat{\mathbf{v}}^2] = [\delta(\mathbf{y}-\hat{\mathbf{x}}),\hat{\mathbf{v}}]\cdot\hat{\mathbf{v}} + \hat{\mathbf{v}}\cdot[\delta(\mathbf{y}-\hat{\mathbf{x}}),\hat{\mathbf{v}}]$ and $[\delta(\mathbf{y}-\hat{\mathbf{x}}),\hat{\mathbf{v}}] = \frac{1}{m}[\delta(\mathbf{y}-\hat{\mathbf{x}}),\hat{\mathbf{p}}] = \frac{i\hbar}{m}\mathrm{grad}_{\mathbf{x}}\delta(\mathbf{y}-\mathbf{x}) = -\frac{i\hbar}{m}\mathrm{grad}_{\mathbf{y}}\delta(\mathbf{y}-\hat{\mathbf{x}})$. Therefore:

$$i\hbar\frac{\partial}{\partial t}\rho(\mathbf{x},t) = -\frac{i\hbar q}{2}\mathrm{grad}_{\mathbf{y}}\cdot U(t,0)\sum_{i=1...N}\delta(\mathbf{y}-\hat{\mathbf{x}}_i)\hat{\mathbf{v}}_i + \hat{\mathbf{v}}_i\delta(\mathbf{y}-\hat{\mathbf{x}}_i)U(t,0)$$

We obtain the continuity equation in operator form:

$$\boxed{\frac{\partial}{\partial t}\rho_H(\mathbf{x},t) = -\mathrm{div}\,\mathbf{J}_H(\mathbf{x},t)}$$

$$\mathbf{J}(\mathbf{x},t) = \frac{q}{2}\sum_{i=1...N}\delta(\mathbf{y}-\hat{\mathbf{x}}_i)\hat{\mathbf{v}}_i + \hat{\mathbf{v}}_i\delta(\mathbf{y}-\hat{\mathbf{x}}_i)$$

We see that the charged current involved in charge conservation is the sum of two terms (the paramagnetic and diamagnetic currents)

$$\mathbf{J}(\mathbf{x},t) = q\,\mathbf{j}(\mathbf{x}) - \frac{q^2}{mc}n(\mathbf{x})\mathbf{A}(\mathbf{x},t)$$

with current for number density $\mathbf{j}(\mathbf{x}) = \frac{1}{2m}\sum_{i=1}^{N}[\hat{\mathbf{p}}_i\delta(\mathbf{x}-\hat{\mathbf{x}}_i) + \delta(\mathbf{x}-\hat{\mathbf{x}}_i)\hat{\mathbf{p}}_i]$. In second quantization:

$$j_\ell(\mathbf{x}) = \frac{i\hbar}{2m}\sum_\mu\left(\frac{\partial\psi_\mu^\dagger}{\partial x^\ell}\psi_\mu - \psi_\mu^\dagger\frac{\partial\psi_\mu}{\partial x^\ell}\right) = \frac{i\hbar}{2m}\left(\frac{\partial}{\partial x^\ell} - \frac{\partial}{\partial y^\ell}\right)\sum_\mu\psi_\mu^\dagger(\mathbf{x})\psi_\mu(\mathbf{y}) \tag{2}$$

and, in the end, $\mathbf{y} = \mathbf{x}$. Note the operator identity $[n(\mathbf{x}),H_0] = -i\hbar\,\mathrm{div}\,\mathbf{j}(\mathbf{x})$.
The Hamiltonian can be re-written in the form:

$$\boxed{H(t) = H_0 - \frac{q}{c}\int d\mathbf{x}\,\mathbf{j}(\mathbf{x})\cdot\mathbf{A}(\mathbf{x},t) + \frac{q^2}{2mc^2}\int d\mathbf{x}\,n(\mathbf{x})\,\mathbf{A}^2(\mathbf{x},t)} \tag{3}$$

where H_0 is the Hamiltonian with $\mathbf{A} = 0$.

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2. Linear response

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

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

In frequency space:

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

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:

$$J_\ell(\mathbf{x},\omega) = \int d\mathbf{x}' \sigma_{\ell m}(\mathbf{x},\mathbf{x}';\omega) E^m(\mathbf{x}',\omega) \tag{4}$$

with conductivity tensor

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

For a homogeneous system the linear relation is

$$\boxed{\mathbf{J}_\ell(\mathbf{k},\omega) = \sigma_{\ell m}(\mathbf{k},\omega)\mathbf{E}^m(\mathbf{k},\omega)} \tag{5}$$

$$\sigma_{\ell m}(\mathbf{k};\omega) = -\frac{e^2}{im\omega} n\delta_{\ell m} - \frac{e^2}{i\hbar\omega} D^{ret}_{\ell m}(\mathbf{k},\omega) \tag{6}$$

For Ohm's law, the real part of conductivity is:

$$\boxed{\sigma_{\ell m}(\mathbf{k};\omega) = -\mathrm{Im}\,\frac{e^2}{\hbar\omega} D^{ret}_{\ell m}(\mathbf{k};\omega)} \tag{7}$$

For a uniform and constant electric field the limits $k \to 0$ and $\omega \to 0$ are taken.

2.1. **The current-current correlator.** A microscopic evaluation requires the correlator

$$-\mathscr{D}_{\ell m}(\mathbf{x},\tau;\mathbf{x}',\tau') = \langle \mathcal{T} \delta j_\ell(\mathbf{x},\tau)\delta j_m(\mathbf{x}',\tau')\rangle_{eq} \tag{8}$$

Insertion of the current densities gives:

$$-\mathscr{D}_{\ell m}(x,x') = \left(\frac{i\hbar}{2m}\right)^2 \sum_{\mu\nu}\left[\frac{\partial}{\partial x_\ell} - \frac{\partial}{\partial y_\ell}\right]\left[\frac{\partial}{\partial x'_m} - \frac{\partial}{\partial y'_m}\right]\left\langle \mathcal{T}\psi^\dagger_\mu(x)\psi_\mu(y)\psi^\dagger_\nu(x')\psi_\nu(y')\right\rangle$$

where, in the end, $y = x$ and $y' = x'$. In the Hartree Fock approximation, we only keep the connected bubble: $\left\langle \mathcal{T}\psi^\dagger_\mu(x)\psi_\mu(y)\psi^\dagger_\nu(x')\psi_\nu(y')\right\rangle \approx -\mathscr{G}_{\mu\nu}(y,x')\mathscr{G}_{\nu\mu}(y',x)$. In a translation-invariant system, and for $\mathscr{G}_{\mu\nu} = \delta_{\mu\nu}\mathscr{G}$:

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

$$\mathscr{D}_{\ell m}(\mathbf{k}, i\nu) = 2\left(\frac{\hbar}{2m}\right)^2 \frac{1}{\hbar\beta}\sum_{i\omega}\int \frac{d\mathbf{q}}{(2\pi)^3}(k_\ell + 2q_\ell)(k_m + 2q_m)\mathscr{G}(\mathbf{k}+\mathbf{q}, i\omega + i\nu)\mathscr{G}(\mathbf{q}, i\omega)$$

Let us insert a spectral representation of the propagator:

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

The Matsubara sum is done and gives:

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

The retarded function is obtained by the replacemet $i\nu \to \nu + i\eta$. Let $\mathbf{k} = 0$:

$$\mathscr{D}^{ret}_{\ell m}(0, \nu) = -\frac{\hbar^2}{2m^2}\int \frac{d\mathbf{q}}{(2\pi)^3} 4q_\ell q_m \int d\omega' d\omega'' A(\mathbf{q}, \omega')A(\mathbf{q}, \omega'')\frac{n(\omega') - n(\omega'')}{\nu - (\omega' - \omega'') + i\eta}$$

The imaginary part is obtained via the Plemelj-Sokhotski formula. The delta function is used to perform one integration:

$$\mathrm{Im}\mathscr{D}^{ret}_{\ell m}(0, \nu) = \frac{4\pi\hbar^2}{2m^2}\int \frac{d\mathbf{q}}{(2\pi)^3} q_\ell q_m \int d\omega A(\mathbf{q}, \omega + \nu)A(\mathbf{q}, \omega)[n(\omega + \nu) - n(\omega)]$$

The ‘static’ limit of conductivity exists:

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

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

$$\sigma(0) = \frac{4\pi e^2}{3\hbar m}\int \frac{d\mathbf{q}}{(2\pi)^3}\frac{\hbar^2 q^2}{2m}\int_{-\infty}^{+\infty} d\omega A^2(q, \omega)\left(-\frac{dn(\omega)}{d\omega}\right) \tag{9}$$

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

$$\sigma(0) = \frac{4\pi e^2}{3m\hbar}\int \frac{d\mathbf{q}}{(2\pi)^3}\epsilon_q\, A^2(q, \frac{\mu}{\hbar}) \approx \frac{4\pi e^2}{3m\hbar}\int_0^\infty d\epsilon\rho(\epsilon)\,\epsilon\, A^2(q, \frac{\mu}{\hbar}) \tag{10}$$

Let us use the following form of spectral function.

$$A(q, \omega) = \frac{1}{2\pi\tau}[(\omega - \tfrac{\epsilon_q}{\hbar})^2 + \tfrac{1}{(2\tau)^2}]^{-1} \tag{11}$$

The integral can be extended to $-\infty$ as the function is evaluated in $\hbar\omega = \mu$ Since the density has slow variation near $\epsilon = \mu$ It is:

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

Note that $\mu\rho(\mu) = \frac{3}{4}n$. A Drude-like formula for direct current (d.c.) conductivity is obtained:

$$\sigma_{d.c.}(0) = \frac{e^2 n}{m}\tau \tag{12}$$

Here τ is the life-time (at Fermi energy) provided by the 1-particle Green function. This is a consequence of the Hartree approximation. However, in linear response the conductivity is a two-particle average.