The Kubo formula of the electric conductivity

We consider an electron under the influence of an electric field $\mathbf{E}(t)$. This system may be described by a Hamiltonian of the form

$$\hat{H}(t) = \hat{H}_0 - e\sum_i E_i(t)x_i, \tag{1}$$

with $\hat{H}_0$ as reference Hamiltonian. For simplicity, we assume a spatially homogeneous field. We further stipulate that $E_i = E_k\delta_{ik}$ and set $ex_k = \hat{D}$. The time evolution of the system is given by the Liouville-von Neumann equation:

$$\frac{\partial\hat{\rho}(t)}{\partial t} = \frac{1}{i\hbar}[\hat{H}(t), \hat{\rho}(t)]. \tag{2}$$

We split the density operator $\hat{\rho}$ into a equilibrium part, $\hat{\rho}_0$, and a time-dependent part $\Delta\hat{\rho}(t)$, according to $(\hat{\rho} = \hat{\rho}_0 + \hat{\Delta}\rho(t))$. We then approximate

$$\frac{\partial\Delta\hat{\rho}}{\partial t} \approx \frac{1}{i\hbar}([\hat{H}_0, \Delta\hat{\rho}(t)] - E_k(t)[\hat{D}, \hat{\rho}_0]. \tag{3}$$

where use has been made of the relation $[\hat{\rho}_0, \hat{H}_0] = 0$. This equation is solved by

$$\Delta\hat{\rho}(t) = -\frac{1}{i\hbar}\int_{-\infty}^{t}[\hat{D}(t'-t), \hat{\rho}_0]E_k(t')dt'. \tag{4}$$

We operate here in the *interaction picture*, implying that $\hat{D}(t) \equiv \hat{U}_0^\dagger(t)\hat{D}\hat{U}_0(t)$, where the propagator $\hat{U}_0(t)$ is defined as $\exp(-\frac{i}{\hbar}\hat{H}_0 t)$. The change in an observable $\hat{O}$ as a function of time can then be found from

$$\Delta O(t) \equiv Tr\{\Delta\hat{\rho}\hat{O}\} = -\frac{1}{i\hbar}\int_{-\infty}^{t}[\hat{D}(t'-t), \hat{\rho}_0]\hat{O}E_k(t')dt' \tag{5}$$

We extend the upper integration limit to positive infinity by introducing the temporally non-local function γ:

$$\gamma_{\hat{O}\hat{D}}(t) = -\frac{1}{i\hbar}\Theta(t)Tr\{[\hat{D}(-t), \hat{\rho}_0]\hat{O}\}, \tag{6}$$

such that

$$\Delta O(t) = \int_{-\infty}^{+\infty}\gamma(t-t')E_k(t')dt' \tag{7}$$

We factorize γ to separate the theta distribution:

$$\gamma_{\hat{O}\hat{D}}(t) = \theta(t)\alpha_{\hat{O}\hat{D}}(t) \tag{8}$$

and observe [1]

$$\alpha_{\hat{O}\hat{D}}(t) = \frac{1}{i\hbar}Tr\{[\hat{\rho}_0, \hat{D}(-t)]\hat{O}\} = \frac{1}{i\hbar}Tr\{\hat{\rho}_0[\hat{D}(-t), \hat{O}]\} = \frac{1}{i\hbar}Tr\{\hat{\rho}_0[\hat{D}(0), \hat{O}(t)]\} \tag{9}$$

In the following step, we identify the operator $\hat{O}$ with the current density operator $\hat{j}_l$. Setting $j_l(t=0)=0$, we obtain from Eqs. (7) - (9):

$$j_l(t) = \int_{-\infty}^{+\infty} \theta(t-t')\alpha_{\hat{O}\hat{D}}(t-t')E_k(t')dt' \tag{10}$$

and

$$\alpha_{\hat{O}\hat{D}}(t-t') = \frac{1}{i\hbar} Tr\{\hat{\rho}_0[\hat{D}(0), \hat{j}_l(t-t')]\}. \tag{11}$$

We find an expression for the conductivity from the Fourier transform of 10, where the Fourier transform of $f(t)$ is defined as $\tilde{f}(\omega) = \int_{-\infty}^{+\infty} f(t)\exp(-i\omega t)dt$, and the back transform as $f(t) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} \tilde{f}(\omega)\exp(i\omega t)d\omega$. Thus

$$\begin{aligned} \tilde{j}_l(\omega) &= \int_{-\infty}^{+\infty} j_l(t)\exp(-i(\omega+i\eta)t)dt \\ &= \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} \Theta(t-t')\alpha_{\hat{O}\hat{D}}(t-t')\exp(-i(\omega+i\eta)(t-t'))dt\, E_k(t')\exp(-i(\omega+i\eta)t')dt' \\ &= \int_{-\infty}^{+\infty} \sigma(\omega)E_k(t')\exp(-i(\omega+i\eta)t')dt'. \end{aligned} \tag{12}$$

We include here an infinitesimal increment $i\eta$ to ensure that the interaction vanishes exponentially as $t, t' \to -\infty$. Summarizing:

$$\tilde{j}_l(\omega) = \tilde{\sigma}_{lk}(\omega)\tilde{E}_k(\omega), \tag{13}$$

with

$$\tilde{E}_k(\omega) = \int_{-\infty}^{+\infty} E_{k0}(t')\exp(-i(\omega+i\eta)t')dt', \tag{14}$$

and

$$\tilde{\sigma}_{lk}(\omega) = \frac{1}{i\hbar}\int_0^{+\infty} Tr\{\hat{\rho}_0[\hat{D}(0), \hat{j}_l(t)]\}\exp(-i(\omega+i\eta)t)dt. \tag{15}$$

We bring the right-hand side of this equation into a more symmetric form, using the relation

$$\tilde{\alpha}_{\hat{A}\hat{B}}(\omega) = \frac{i}{\omega}\tilde{\alpha}_{\hat{C}\hat{B}}(\omega), \tag{16}$$

where

$$\hat{C}(t) = \frac{d\hat{A}}{dt}(t). \tag{17}$$

To justify this result, we operate with the complete bases $|m\rangle\langle m|$ and $|n\rangle\langle n|$, and set

$$\hat{\rho}_0 = |m\rangle p_m \langle m|. \tag{18}$$

Thus, we have

$$\alpha_{\hat{A}\hat{B}}(t) = \frac{1}{i\hbar}\sum_{m,n} p_m (A_{mn}B_{nm}e^{-i\omega_{mn}t} - B_{nm}A_{mn}e^{i\omega_{mn}t}), \tag{19}$$

where $\omega_{mn} \equiv \frac{(E_m - E_n)}{\hbar}$. For the Fourier transform of $\alpha_{\hat{A}\hat{B}}(t)$ we find

$$\tilde{\alpha}_{\hat{A}\hat{B}}(\omega) = \frac{2\pi}{i\hbar}\sum_{m,n} p_m (A_{mn}B_{nm}\delta(\omega + \omega_{mn}) - B_{mn}A_{nm}\delta(\omega - \omega_{mn})). \tag{20}$$

If $\hat{C} = \frac{d\hat{A}}{dt} = \frac{1}{i\hbar}[\hat{A}, \hat{H}_0]$, then

$$\tilde{\alpha}_{\hat{C}\hat{B}}(\omega) = \frac{2\pi}{i}\sum_{m,n} p_m (-\omega_{nm}A_{mn}B_{nm}\delta(\omega + \omega_{mn}) - \omega_{mn}B_{mn}A_{nm}\delta(\omega - \omega_{mn})), \tag{21}$$

from which we obtain Eq.(16).

We identify $\hat{A}$ with the dipole moment operator and derive the following relation between $\hat{D}$ and $\hat{j}_k$:

$$\hat{j}_k(t) = \frac{1}{a^d}\frac{d\hat{D}}{dt}(t). \tag{22}$$

where a^d is the d-dimensional real space volume per particle. As we use Eq. (17) to substitute for $\hat{D}(0)$ in Eq. (15), we obtain:

$$\tilde{\sigma}_{lk}(\omega) = \frac{a^d}{\hbar\omega}\int_0^{+\infty} Tr\{\hat{\rho}_0[\hat{j}_k(0), \hat{j}_l(t)]\} \exp(-i(\omega + i\eta)\ t)dt. \tag{23}$$

This expression for $\sigma_{lk}(\omega)$ is referred to as *Kubo's formula of conductivity.* Using the identity

$$\hat{j}_l = \frac{e}{a^d}\hat{v}_l, \tag{24}$$

with

$$\hat{v}_l = \frac{i}{\hbar}[\hat{H}, x_l] = \frac{i}{\hbar}[\hat{H}_0, x_l] \tag{25}$$

we express the current density operators $\hat{\mathbf{j}}$ through velocity operators $\hat{\mathbf{v}}$. Further, we consider the transverse conductance in the two-dimensional case,$d = 2$, as relevant for the quantum Hall effect in a graphene sheet. With $k = x$ and $l = y$, this yields:

$$\tilde{\sigma}_{xy}(\omega) = \frac{e^2}{\hbar\omega a^2}\int_0^{+\infty} Tr\{\hat{\rho}_0[\hat{v}_x(0), \hat{v}_y(t)]\}\exp(-i(\omega+i\eta)t)dt. \tag{26}$$

In order to carry out the trace, we adopt the basis $\{|m\rangle\}$, where

$$\hat{H}_0|m\rangle = E_m|m\rangle. \tag{27}$$

We note that

$$\hat{\rho}_0|m\rangle = F(E_m)|m\rangle, \tag{28}$$

where F denotes the Fermi-Dirac distribution, and

$$\langle n|\hat{v}_y(t)|m\rangle = \langle n|\hat{U}_0^\dagger(t)\hat{v}_y\hat{U}_0(t)|m\rangle = \exp(-\frac{i}{\hbar}(E_m - E_n)t)\langle n|\hat{v}_y|m\rangle. \tag{29}$$

With the help of the latter statements, and after inserting a complete basis $|n\rangle\langle n| = \hat{1}$ between the operators $\hat{v}_x$ and $\hat{v}_y$, the integration in Eq. (26) can be performed directly. This results in [2]

$$\tilde{\sigma}_{xy}(\omega) = \frac{e^2}{i\omega a^d}\sum_{m,n}(F(E_m) - F(E_n))\frac{\langle m|\hat{v}_x|n\rangle\langle n|\hat{v}_y|m\rangle}{\hbar\omega + i\hbar\eta + E_m - E_n}. \tag{30}$$

Expanding $\frac{1}{\hbar\omega+i\hbar\eta+E_m-E_n}$ up to first order with respect to $\hbar\omega$, we obtain

$$\tilde{\sigma}_{xy}(\omega) = \frac{i\hbar e^2}{a^d}\sum_{m,n}(F(E_m) - F(E_n))\frac{\langle m|\hat{v}_x|n\rangle\langle n|\hat{v}_y|m\rangle}{\hbar\omega - i\hbar\eta + E_m - E_n}. \tag{31}$$

Note that the zeroth-order term of this expansion does not contribute, as the sum over m, n vanishes for this contribution. Considering the DC conductivity ($\omega = 0$) at zero temperature, and setting $\eta = 0$, we find

$$\tilde{\sigma}_{xy}(\omega) = \frac{i\hbar e^2}{a^d}\sum_{m,n}(\Theta(E_F - E_m) - \Theta(E_F - E_n))\frac{\langle m|\hat{v}_x|n\rangle\langle n|\hat{v}_y|m\rangle}{(E_m - E_n)^2}. \tag{32}$$

The factor following the summation sign is non-zero only if $E_m < E_F < E_n$ or $E_n < E_F < E_m$. Summing over these two configurations results in

$$\tilde{\sigma}_{xy} = \frac{i\hbar e^2}{a^d}\sum_{E_m<E_F, E_n>E_F}\frac{\langle m|\hat{v}_x|n\rangle\langle n|\hat{v}_y|m\rangle - \langle m|\hat{v}_y|n\rangle\langle n|\hat{v}_x|m\rangle}{(E_m - E_n)^2}. \tag{33}$$

In the following, we focus on electronic states in lattices, as described by Bloch functions (see (3.116)), assuming $|m\rangle, |n\rangle$ to be located in the first Brillouin zone. From Eq. (25), we conclude

$$\langle n|\hat{v}_i|m\rangle = \frac{\langle n|x_i\hat{H}_0|m\rangle - \langle n|\hat{H}_0 x_i|m\rangle}{i\hbar} = \frac{E_m - E_n}{i\hbar}\langle n|x_i|m\rangle = \frac{E_m - E_n}{\hbar}\langle n|\frac{\partial}{\partial k_i}|m\rangle, \tag{34}$$

where $i = x, y$. Likewise:

$$\langle m|\hat{v}_i|n\rangle = -\frac{E_n - E_m}{\hbar}\langle\frac{\partial}{\partial k_i}m|n\rangle. \tag{35}$$

The latter relation involves a shift of the derivative $\frac{\partial}{\partial k_i}$ from the ket to the bra position of the scalar product. This is legitimate, as the position operator in k-space ($=i\frac{\partial}{\partial k_i}$) is hermitian in the region considered here, namely a Brillouin zone, and thus a space with periodic boundary conditions. By Eqs. (34) and (35), it holds that

$$\tilde{\sigma}_{xy} = \frac{ie^2}{\hbar a^d}\sum_{E_m<E_F, E_n>E_F}\langle\frac{\partial}{\partial k_x}m|n\rangle\langle n|\frac{\partial}{\partial k_y}m\rangle - \langle\frac{\partial}{\partial k_y}m|n\rangle\langle n|\frac{\partial}{\partial k_x}m\rangle. \tag{36}$$

The sum over the unoccupied states can be expressed through the sum over the occupied states by employing the completeness relation:

$$\sum_{E_n>E_F}|n\rangle\langle n| = \mathbf{1} - \sum_{E_n<E_F}|n\rangle\langle n|. \tag{37}$$

Transforming Eq. (36) by use of the identity (37) we find [3]

$$\tilde{\sigma}_{xy} = \frac{ie^2}{\hbar a^d}\sum_{\mathbf{k}}\sum_{E_m<E_F}\langle\frac{\partial}{\partial k_x}m|\frac{\partial}{\partial k_y}m\rangle - \langle\frac{\partial}{\partial k_y}m|\frac{\partial}{\partial k_x}m\rangle. \tag{38}$$

The contribution to $\tilde{\sigma}_{xy}$ due to the second term on the right-hand side of Eq. (37) yields an expression that is odd with respect to the exchange of the indices m and n and thus vanishes upon summing over these indices. In what follows, we will consider the two-dimensional case which is of relevance for the planar graphene sheet. In order to take formula (38) into its ultimate form we make two further steps. First, we average the conductivity as given by Eq. (38) over the first Brillouin zone (BZ), involving integration with respect to k_x, k_y over the Brillouin zone while simultaneously dividing through its area, $\frac{(2\pi)^2}{a^d}$ [1]:

$$\tilde{\sigma}_{xy}^{BZ} = \frac{ie^2}{h}\int_{BZ}\frac{dk_x dk_y}{2\pi}\sum_{E_m<E_F}\langle\frac{\partial}{\partial k_x}m|\frac{\partial}{\partial k_y}m\rangle - \langle\frac{\partial}{\partial k_y}m|\frac{\partial}{\partial k_x}m\rangle. \tag{39}$$

Secondly, we introduce the vector field $\mathbf{A}_{\mathbf{k}}$ by defining

[1]Each k-space area cell contributes $\frac{dk_x dk_y}{(2\pi)^2}$ to the electron density, see p.91 of the main text.

$$A_{\mathbf{k},x} = i \sum_{E_m < E_F} \langle m | \frac{\partial}{\partial k_x} m \rangle, A_{\mathbf{k},y} = i \sum_{E_m < E_F} \langle m | \frac{\partial}{\partial k_y} m \rangle. \qquad (40)$$

Substituting Eq. (40) into Eq. (39), we find

$$\tilde{\sigma}_{xy}^{BZ} = \frac{e^2}{h} \int_{BZ} \frac{dk_x dk_y}{2\pi} [\frac{\partial}{\partial k_x} A_{\mathbf{k},y} - \frac{\partial}{\partial k_y} A_{\mathbf{k},x}]. \qquad (41)$$

or, dropping the superscript BZ:

$$\tilde{\sigma}_{xy} = \frac{e^2}{h} \int_{BZ} \frac{dk_x dk_y}{2\pi} (\nabla_{\mathbf{k}} \times \mathbf{A}_{\mathbf{k}})_z. \qquad (42)$$

By use of Stoke's theorem, the right-hand side may be expressed as a line integral over the contour of the first Brillouin zone:

$$\tilde{\sigma}_{xy} = \frac{e^2}{2\pi h} \oint d\mathbf{k}\, \mathbf{A}_{\mathbf{k}}. \qquad (43)$$

Bibliography

[1] T.O.Stadelmann, *Antidot Superlattices in InAsGaSb Double Heterostructures: Transport Studies*, Ph.D. Thesis, Oxford 2006.

[2] G.Tkachov, *Topological Insulators*, Pan Stanford Publishing, 2016

[3] D.J.Thouless, M.Kohmoto, M.P.Nightingale, M.de Nijs, Phys.Rev.Lett.49, 405 (1982)