B Calculating Conductivity

> The mathematics is not there till we put it there.
>
> *(Sir Arthur Stanley Eddington, The Philosophy of Physical Science)*

B.1 The Boltzmann Equation

The Boltzmann Equation describes, in the presence of scattering, the evolution of the distribution function $f(\mathbf{r}, \mathbf{k}, t)$ of an ensemble of particles obeying the semiclassical equations of motion

$$\dot{\mathbf{r}} = \mathbf{v}(\mathbf{k}) \qquad \text{and} \tag{B.1}$$

$$\hbar\dot{\mathbf{k}} = \mathbf{F}(\mathbf{r}, \mathbf{k}), \tag{B.2}$$

where $\mathbf{r}(t)$ and $\mathbf{k}(t)$ denote position and crystal momentum, and $\mathbf{v}$ and $\mathbf{F}$ have their usual meanings of velocity and force, respectively. It can then be shown that [1]

$$\frac{df(\mathbf{r}, \mathbf{k}, t)}{dt} = \left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{r}} + \mathbf{F} \cdot \frac{1}{\hbar} \nabla_{\mathbf{k}}\right) f(\mathbf{r}, \mathbf{k}, t) = \left[\frac{\partial f(\mathbf{r}, \mathbf{k}, t)}{\partial t}\right]_{\text{coll}}, \tag{B.3}$$

where the right hand side describes the change in $f(\mathbf{r}, \mathbf{k}, t)$ due to collisions.

Once $f(\mathbf{r}, \mathbf{k}, t)$ is known, the carrier and current densities can be calculated by integrating over momentum space, yielding

$$n(\mathbf{r}, t) = (2\pi)^{-d} \int g(\mathbf{k}) f(\mathbf{r}, \mathbf{k}, t)\, d\mathbf{k} \qquad \text{and} \tag{B.4}$$

$$\mathbf{j}(\mathbf{r}, t) = (2\pi)^{-d} \int g(\mathbf{k}) f(\mathbf{r}, \mathbf{k}, t) q \mathbf{v}(\mathbf{k})\, d\mathbf{k}, \tag{B.5}$$

where d is the number of dimensions and $g(\mathbf{k})$ is the density of states.

To make the Boltzmann equation (B.3) tractable, the relaxation time approximation is often used. It amounts to the assumption that the scattering probability for a carrier with momentum $\mathbf{k}$ at position $\mathbf{r}$ is of the form $dt/\tau(\mathbf{r},\mathbf{k})$, and that the distribution of carriers emerging from collisions is the local equilibrium distribution $f_0(\mathbf{r},\mathbf{k},t)$, *i.e.*, the Fermi-Dirac distribution $f_{\mathrm{FD}}(E) \overset{\mathrm{def}}{=} \{\exp[(E-\mu)/k_{\mathrm{B}}T]+1\}^{-1}$ evaluated at $E = E[\mathbf{k}(t)]$ and allowing for a local temperature $T = T[\mathbf{r}(t)]$ and chemical potential $\mu = \mu[\mathbf{r}(t)]$. The collision term then has the simple form

$$\left[\frac{\partial f(\mathbf{r},\mathbf{k},t)}{\partial t}\right]_{\mathrm{coll}} = -\frac{f(\mathbf{r},\mathbf{k},t) - f_0(\mathbf{r},\mathbf{k},t)}{\tau(\mathbf{r},\mathbf{k})}, \tag{B.6}$$

and the Boltzmann equation (B.3) becomes

$$\frac{df(\mathbf{r},\mathbf{k},t)}{dt} = -\frac{f(\mathbf{r},\mathbf{k},t) - f_0(\mathbf{r},\mathbf{k},t)}{\tau(\mathbf{r},\mathbf{k})}. \tag{B.7}$$

Eq. (B.7) can be now be solved using standard techniques, leading to

$$f(\mathbf{r},\mathbf{k},t) = e^{-\int \tau(\mathbf{r},\mathbf{k})^{-1}\,dt}\left(\int_{-\infty}^{t} \frac{f_0(\mathbf{r},\mathbf{k},t)\,e^{\int \tau(\mathbf{r},\mathbf{k})^{-1}\,dt}}{\tau(\mathbf{r},\mathbf{k})}\,dt + \text{const.}\right). \tag{B.8}$$

The constant (with respect to t) depends on the initial conditions and the corresponding term decays exponentially for physical $\tau(\mathbf{r},\mathbf{k})$. The first term, which describes the intrinsic behaviour of the system, may also be written as [1]

$$f(\mathbf{r},\mathbf{k},t) = f_0(\mathbf{r},\mathbf{k},t) - \int_{-\infty}^{t} P(t,t')\frac{d}{dt'}f_0(\mathbf{r},\mathbf{k},t)\,dt', \tag{B.9}$$

where $P(t,t') \overset{\mathrm{def}}{=} \exp\{-\int_{t'}^{t} 1/\tau[\mathbf{r}(t''),\mathbf{k}(t'')]\,dt''\}$ is the probability for a particle with momentum $\mathbf{k}(t)$ at position $\mathbf{r}(t)$ *not* to have undergone collision in the time interval $[t',t]$.

If $\mathbf{v}(\mathbf{k}) = (1/\hbar)\,\nabla_{\mathbf{k}} E(\mathbf{k})$, the force is $\mathbf{F}(\mathbf{r},\mathbf{k}) = q[\mathbf{E}(\mathbf{r},t)+\mathbf{v}(\mathbf{k})\times\mathbf{B}(\mathbf{r},t)]$, and the chemical potential μ as well as the temperature T are independent of position, then

$$\frac{df_0(\mathbf{r},\mathbf{k},t)}{dt} = \frac{\partial f_0(\mathbf{r},\mathbf{k},t)}{\partial E}\,\hbar\mathbf{v}(\mathbf{k})\cdot\frac{q\mathbf{E}(\mathbf{r},t)}{\hbar} = q\frac{\partial f_{\mathrm{FD}}(E)}{\partial E}\,\mathbf{v}(\mathbf{k})\cdot\mathbf{E}(\mathbf{r},t); \tag{B.10}$$

if one also makes the simplifying assumption of a constant relaxation time τ,[1] $P(t,t') = \exp[-(t-t')/\tau]$. Under these conditions, Eq. (B.9) becomes

$$f(\mathbf{r},\mathbf{k},t) = f_0(\mathbf{r},\mathbf{k},t) - q\int_{-\infty}^{t} e^{-(t-t')/\tau}\frac{\partial f_{\mathrm{FD}}(E)}{\partial E}\mathbf{v}(\mathbf{k})\cdot\mathbf{E}(\mathbf{r},t)\,dt', \tag{B.11}$$

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[1] If τ only depends on energy, $\partial\tau/\partial t$ is still approximately zero in metals and the same arguments can be used [1].

which further simplifies to

$$f(\mathbf{k}) = f_0(\mathbf{k}) - \Re\left[\frac{q}{\tau^{-1} - i\omega}\frac{\partial f_{\mathrm{FD}}(E)}{\partial E}\mathbf{v}(\mathbf{k}) \cdot \mathbf{E}(\omega)\right] \tag{B.12}$$

if $\mathbf{B}(\mathbf{r}, t) = \mathbf{0}$ and $\mathbf{E}(\mathbf{r}, t) = \Re[\mathbf{E}(\omega)\exp(-i\omega t)]$. Using Eq. (B.12) in Eq. (B.5), the current density $\mathbf{j}(\omega)$ is calculated as

$$\mathbf{j}(\omega) = \frac{q^2}{(2\pi)^d}\int \frac{g(E)}{\tau^{-1} - i\omega}\frac{\partial f_{\mathrm{FD}}(E)}{\partial E}\mathbf{v}(\mathbf{k}) \cdot \mathbf{E}(\omega)\,\mathbf{v}(\mathbf{k})\,d\mathbf{k}. \tag{B.13}$$

Since $\mathbf{j}(\omega) = \boldsymbol{\sigma}(\omega)\mathbf{E}(\omega)$, the conductivity tensor is accordingly

$$\sigma_{\mu\nu}(\omega) = \frac{q^2}{(2\pi)^d}\int \frac{g(E)}{\tau^{-1} - i\omega}\left[-\frac{\partial f_{\mathrm{FD}}(E)}{\partial E}\right]v_\mu(\mathbf{k})v_\nu(\mathbf{k})\,d\mathbf{k}. \tag{B.14}$$

The derivation is independently valid for every energy band in which $\partial f_{\mathrm{FD}}(E)/\partial E$ is non-zero (*i.e.*, which intersects the Fermi level), and the total conductivity is obtained by summing the contributions of all such bands multiplied by their individual degeneracies.

B.2 Kubo's Linear Response Theory

B.2.1 Fundamentals

In his 1957 paper [2], Ryogo Kubo discusses how the linear response to a small perturbation of a system in equilibrium can be expressed in terms of the fluctuations of dynamical variables of the unperturbed system. His linear response theory, which extended and unified prior work on the statistical description of transport properties, has since become an important tool in fields such as condensed matter physics and fluid dynamics.

If $B(t)$ is a physical quantity corresponding to the expectation value of an observable $\hat{B}$ at time t, the linear change $\Delta B(t)$ in $B(t)$ due to a spatially homogeneous[2] field $\xi_A(t)$ can be written as

$$\Delta B(t) = \int_{-\infty}^{\infty} \alpha_{BA}(t - t')\xi(t')\,dt', \tag{B.15}$$

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[2] The generalization to inhomogeneous fields is complicated, but conceptually straightforward.

where $\alpha_{BA}(t)$ is the response at time t caused by a unit impulse at $t = 0$, and causality implies $\alpha_{BA}(t) = 0$ for $t < 0$. For a periodic field $\xi_A(t) = \Re\big[\xi_A^{(0)} \exp(i\omega t)\big]$, the response is expressed as

$$\Delta B_\omega(t) = \Re\left[\chi_{BA}(\omega)\xi_A^{(0)} e^{i\omega t}\right], \tag{B.16}$$

where the complex susceptibility $\chi_{BA}(\omega)$ is the Fourier transform of $\alpha_{BA}(t)$.[3]

To calculate $\alpha_{BA}(t)$, Kubo assumes that the system is described by the Hamiltonian $\hat{H}(t) = \hat{H}_0 - \xi_A(t)\hat{A}$, where $\hat{H}_0$ governs the natural motion of the unperturbed system and $\hat{A}$ is the generalized force conjugate to $\xi_A(t)$. The density matrix $\rho(t)$ then obeys the equation

$$\frac{\partial\rho(t)}{\partial t} = \frac{1}{i\hbar}\big[\hat{H}(t), \rho(t)\big] = \frac{1}{i\hbar}\big(\big[\hat{H}_0, \rho(t)\big] - \xi_A(t)\big[\hat{A}, \rho(t)\big]\big). \tag{B.17}$$

With the *Ansatz* $\rho(t) = \rho_0 + \Delta\rho(t)$, where $\Delta\rho(t) \to 0$ as $t \to -\infty$ and ρ_0 is taken to be the equilibrium distribution, *i.e.*, $[\rho_0, \hat{H}_0] = 0$, he simplifies Eq. (B.17) to

$$\frac{\partial\Delta\rho(t)}{\partial t} \approx \frac{1}{i\hbar}\big(\big[\hat{H}_0, \Delta\rho(t)\big] - \xi_A(t)\big[\hat{A}, \rho_0\big]\big), \tag{B.18}$$

which can be solved for $\Delta\rho(t)$ [2,3], giving

$$\Delta\rho(t) = -\frac{1}{i\hbar}\int_{-\infty}^{t} \big[\hat{A}(t'-t), \rho_0\big]\xi_A(t')\, dt', \tag{B.19}$$

where $\hat{A}(t) \overset{\text{def}}{=} \hat{U}_0^\dagger(t)\hat{A}\hat{U}_0(t)$ is a Heisenberg operator constructed using the time evolution operator $\hat{U}_0(t) \overset{\text{def}}{=} \exp(-i\hat{H}_0 t/\hbar)$. From Eq. (B.19) $\Delta B(t)$ follows as

$$\Delta B(t) = \operatorname{Tr}\Delta\rho(t)\hat{B} = -\frac{1}{i\hbar}\int_{-\infty}^{t} \operatorname{Tr}\big[\hat{A}(t'-t), \rho_0\big]\hat{B}\xi_A(t')\, dt'. \tag{B.20}$$

Comparing Eqs. (B.15) and (B.20), one finds

$$\alpha_{BA}(t) = \theta(t)\varphi_{BA}(t), \tag{B.21}$$

where $\theta(t)$ is the Heaviside function and

$$\varphi_{BA}(t) = -\frac{1}{i\hbar}\operatorname{Tr}\big[\hat{A}(-t), \rho_0\big]\hat{B}. \tag{B.22}$$

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[3] In the following I shall define the Fourier transform of $F(t)$ as $\tilde{F}(\omega) \overset{\text{def}}{=} \int_{-\infty}^{\infty} F(t)\exp(-i\omega t)\, dt$ so that $F(t) = (1/2\pi)\int_{-\infty}^{\infty} \tilde{F}(\omega)\exp(i\omega t)\, d\omega$.

Because of the cyclic property of the trace and the definition of the Heisenberg operators, Eq. (B.22) can be rewritten as

$$\begin{aligned}
\varphi_{BA}(t) &= \frac{1}{i\hbar}\operatorname{Tr}\big[\rho_0, \hat{A}(-t)\big]\hat{B} \\
&= \frac{1}{i\hbar}\operatorname{Tr}\rho_0\big[\hat{A}(-t), \hat{B}\big] \\
&= \frac{1}{i\hbar}\operatorname{Tr}\rho_0\big[\hat{A}(0), \hat{B}(t)\big] \qquad \text{(B.23)} \\
&= \frac{1}{i\hbar}\big\langle\big[\hat{A}(0), \hat{B}(t)\big]\big\rangle_0 . \qquad \text{(B.24)}
\end{aligned}$$

An analogous expression is found in the classical case; the derivation proceeds along exactly the same lines if ρ is taken as the classical phase space distribution function, the commutator $(1/i\hbar)[\hat{A}, \hat{B}]$ is replaced by the classical Poisson bracket $(A, B) \overset{\text{def}}{=} \sum_i \big[(\partial A/\partial q_i)(\partial B/\partial p_i) - (\partial A/\partial p_i)(\partial B/\partial q_i)\big]$ and the trace by integration over the full set $\{p_i, q_i\}$ of phase space coordinates.

In terms of matrix elements $A_{mn} \overset{\text{def}}{=} \langle m|\hat{A}|n\rangle$ in the basis of the eigenstates $|n\rangle$ of $\hat{H}_0$, the response function Eq. (B.24) is given explicitly as

$$\varphi_{BA}(t) = \frac{1}{i\hbar}\sum_{n,m} p_n \left(A_{nm}B_{mn}e^{-i\omega_{nm}t} - B_{nm}A_{mn}e^{i\omega_{nm}t}\right), \qquad \text{(B.25)}$$

where p_n are the weights of the density matrix $\rho_0 = \sum_n |n\rangle\, p_n\, \langle m|$, I define $\omega_{nm} \overset{\text{def}}{=} (E_n - E_m)/\hbar$, and E_n are the eigenvalues of $\hat{H}_0$. In the same basis, the Fourier transform of $\varphi_{AB}(t)$ is written as

$$\begin{aligned}
\tilde{\varphi}_{BA}(\omega) &= \frac{2\pi}{i\hbar}\sum_{n,m} p_n\big[A_{nm}B_{mn}\delta(\omega + \omega_{nm}) - B_{nm}A_{mn}\delta(\omega - \omega_{nm})\big] \qquad \text{(B.26)} \\
&= \frac{2\pi}{i\hbar}\sum_{n,m}(p_n - p_m)A_{nm}B_{mn}\delta(\omega + \omega_{nm}). \qquad \text{(B.27)}
\end{aligned}$$

B.2.2 Correlation Functions

To relate them to physically meaningful quantities, it is convenient to express $\tilde{\varphi}_{BA}(\omega)$—and hence $\varphi_{BA}(t)$, $\alpha_{BA}(t)$, and $\chi_{BA}(\omega)$—in terms of the symmetrized correlation function

$$\Psi_{BA}(t) \overset{\text{def}}{=} \big\langle\big\{\hat{A}(0), \hat{B}(t)\big\}\big\rangle_0 \overset{\text{def}}{=} \frac{1}{2}\big\langle\hat{A}(0)\hat{B}(t) + \hat{B}(t)\hat{A}(0)\big\rangle_0 , \qquad \text{(B.28)}$$

which is one of the possible quantum mechanical equivalents of the classical correlation function $\langle A(0)B(t)\rangle$. In the basis of the energy eigenstates, the symmetrized correlation function becomes

$$\Psi_{BA}(t) = \frac{1}{2}\sum_{n,m} p_n\left(A_{nm}B_{mn}e^{-i\omega_{nm}t} + B_{nm}A_{mn}e^{i\omega_{nm}t}\right) \qquad \text{and} \tag{B.29}$$

$$\tilde{\Psi}_{BA}(\omega) = \pi\sum_{n,m} p_n\big[A_{nm}B_{mn}\delta(\omega+\omega_{nm}) + B_{nm}A_{mn}\delta(\omega-\omega_{nm})\big] \tag{B.30}$$

$$= \pi\sum_{n,m}(p_n+p_m)A_{nm}B_{mn}\delta(\omega+\omega_{nm}). \tag{B.31}$$

If $\rho_0 = \rho_0^{(\beta)}$ is a canonical distribution at the temperature $T = 1/k_\mathrm{B}\beta$ [2, 4], the weights are $p_n = \exp(-\beta E_n)/\sum_m \exp(-\beta E_m)$ and $(p_n - p_m)/(p_n + p_m) = \tanh[-\frac{1}{2}\beta(E_n - E_m)]$. Eq. (B.27) then becomes

$$\begin{aligned}\tilde{\varphi}^{(\beta)}_{BA}(\omega) &= \frac{2\pi}{i\hbar}\sum_{n,m}\tanh\!\left(\frac{1}{2}\beta\hbar\omega_{nm}\right)(p_n+p_m)A_{nm}B_{mn}\delta(\omega+\omega_{nm}) \\ &= \frac{2}{i\hbar}\tanh\!\left(\frac{1}{2}\beta\hbar\omega\right)\tilde{\Psi}^{(\beta)}_{BA}(\omega) = \frac{\omega}{iE_\beta(\omega)}\tilde{\Psi}^{(\beta)}_{BA}(\omega),\end{aligned} \tag{B.32}$$

where $E_\beta(\omega) = \hbar\omega/2 + \hbar\omega/[\exp(\beta\hbar\omega) - 1]$ is the average energy of an harmonic oscillator with frequency ω at $T = 1/k_\mathrm{B}\beta$. On the other hand, if $\rho_0 = \rho_0^{(\mathrm{mp})}$ describes a system of many non-interacting particles [4], we can write the $\tilde{\varphi}^{(\mathrm{mp})}_{BA}(\omega)$ and $\tilde{\Psi}^{(\mathrm{mp})}_{BA}(\omega)$ in terms of the single particle microcanonical spectra $\tilde{\varphi}^{(E)}_{BA}(\omega)$ and $\tilde{\Psi}^{(E)}_{BA}(\omega)$ as

$$\tilde{\varphi}^{(\mathrm{mp})}_{BA}(\omega) = \sum_n p_n\tilde{\varphi}^{(E_n)}_{BA}(\omega) \qquad \text{and} \qquad \tilde{\Psi}^{(\mathrm{mp})}_{BA}(\omega) = \sum_n p_n\tilde{\Psi}^{(E_n)}_{BA}(\omega), \tag{B.33}$$

where $\tilde{\varphi}^{(E_n)}_{BA}(\omega)$ and $\tilde{\Psi}^{(E_n)}_{BA}(\omega)$ can be identified by comparing Eq. (B.33) with Eqs. (B.26) and (B.30). By exchanging summation indices in Eq. (B.26), adding the permutated version to the original, and dividing by 2, we can write

$$\begin{aligned}\tilde{\varphi}^{(\mathrm{mp})}_{BA}(\omega) &= \frac{\pi}{i\hbar}\sum_{n,m}(p_n-p_m)\big[A_{nm}B_{mn}\delta(\omega+\omega_{nm}) - B_{nm}A_{mn}\delta(\omega-\omega_{nm})\big] \\ &= -\omega\frac{\pi}{i}\sum_{n,m}\frac{p_n-p_m}{E_n-E_m}\big[A_{nm}B_{mn}\delta(\omega+\omega_{nm}) + B_{nm}A_{mn}\delta(\omega-\omega_{nm})\big].\end{aligned} \tag{B.34}$$

If $f(E_n) \overset{\text{def}}{=} p_n$ and the level spacing $\hbar\omega_{nm}$ is small, so that $\left[f(E_n) - f(E_m)\right] \big/ (E_n - E_m) \approx \partial f_{\text{FD}}(E_n)/\,\partial E_n$ independent of m, Eq. (B.34) becomes

$$\tilde{\varphi}^{(\text{mp})}_{BA}(\omega) = -\frac{\omega}{i}\sum_n \frac{\partial f_{\text{FD}}(E_n)}{\partial E_n}\tilde{\Psi}^{(E_n)}_{BA}(\omega). \tag{B.35}$$

In the same limit of small $\hbar\omega_{nm}$ (and specifically if the density of states $g(E)$ is well defined) the sum over n can be replaced by integration over energy, leading to

$$\tilde{\varphi}^{(\text{mp})}_{BA}(\omega) = \int_0^\infty L^d g(E) f(E)\tilde{\varphi}^{(E)}_{BA}(\omega)\,dE = -\frac{\omega}{i}\int_0^\infty L^d g(E)\frac{\partial f_{\text{FD}}(E)}{\partial E}\tilde{\Psi}^{(E)}_{BA}(\omega)\,dE, \tag{B.36}$$

where L^d is the d-dimensional real space volume per particle, so that $L^d g(E)$ is the energy density of single-particle states.

B.2.3 Electrical Conduction

Kubo's linear response theory is directly applicable to the problem of electrical conduction. The complex conductivity tensor $\sigma_{\mu\nu}(\omega)$ relates the current density $J_\mu(t)$ in the μ-direction to the electric field $E_\nu(t) = \Re\big[E^{(0)}_\nu \exp(i\omega t)\big]$ in the ν-direction and obeys the relation

$$J_\mu(t) = \Re\left[\sigma_{\mu\nu}(\omega)E^{(0)}_\nu e^{i\omega t}\right]. \tag{B.37}$$

If $\hat{H} = \hat{H}_0 - \sum_i q_i \sum_\nu E_\nu(t)\hat{r}^{(i)}_\nu$ is the Hamiltonian of a system consisting of many particles with charges q_i and position operators $\hat{\mathbf{r}}^{(i)}$, while $\hat{A}$ is the polarization $\hat{\Pi}_\nu \overset{\text{def}}{=} \sum_i q_i \hat{r}^{(i)}_\nu$, Eqs. (B.16), (B.21) and (B.24) imply

$$\begin{aligned}
\sigma_{\mu\nu}(\omega) &= \frac{1}{i\hbar}\int_0^\infty \left\langle\left[\hat{\Pi}_\nu(0), \hat{J}_\mu(t)\right]\right\rangle_0 e^{-i\omega t}\,dt && \text{(B.38)}\\
&= \frac{V}{\hbar\omega}\int_0^\infty \left\langle\left[\hat{J}_\nu(0), \hat{J}_\mu(t)\right]\right\rangle_0 e^{-i\omega t}\,dt, && \text{(B.39)}
\end{aligned}$$

where V is the total volume of the system. The last step follows from $\hat{J} = \dot{\hat{\Pi}}/V$, where $\dot{\hat{\Pi}} \overset{\text{def}}{=} (1/i\hbar)\big[\hat{\Pi}(t), \hat{H}_0\big]$, and the fact that $\tilde{\varphi}_{AB}(\omega) = (i/\omega)\tilde{\varphi}_{CB}(\omega)$ if $\hat{C}(t) = \dot{\hat{A}}(t)$.[4] If the system is in thermal equilibrium with a heat reservoir, by Eq. (B.32)

$$\sigma_{\mu\nu}(\omega) = \frac{V}{E_\beta(\omega)}\int_0^\infty \left\langle\left\{\hat{J}_\nu(0), \hat{J}_\mu(t)\right\}\right\rangle^{(\beta)}_0 e^{-i\omega t}\,dt, \tag{B.40}$$

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[4] This can be verified by expressing both sides in terms of matrix elements.

which is one of the results commonly referred to as the *'Kubo formula'* of conductivity.[5] For non-interacting electrons, Eq. (B.39) becomes

$$\sigma_{\mu\nu}(\omega) = \frac{e^2}{\hbar\omega L^d} \int_0^\infty \left\langle \left[\hat{v}_\nu(0), \hat{v}_\mu(t) \right] \right\rangle_0^{(\mathrm{F})} e^{-i\omega t}\, dt \tag{B.41}$$

$$= \frac{e^2\hbar}{iL^d} \sum_{n,m} \frac{f_{\mathrm{FD}}(E_n) - f_{\mathrm{FD}}(E_m)}{E_n - E_m} \frac{\langle n|\hat{v}_\nu|m\rangle \langle m|\hat{v}_\mu|n\rangle}{\hbar\omega + (E_n - E_m) + i0^+} \tag{B.42}$$

where $f_{\mathrm{FD}}(E)$ is the Fermi-Dirac distribution. If the requirements for Eq. (B.36) are met, we may further approximate Eq. (B.41) as

$$\sigma_{\mu\nu}(\omega) = e^2 \int_0^\infty dE \int_0^\infty dt\; g(E) \left[-\frac{\partial f_{\mathrm{FD}}(E)}{\partial E} \right] \left\langle \left\{ \hat{v}_\nu(0), \hat{v}_\mu(t) \right\} \right\rangle_0^{(E)} e^{-i\omega t}. \tag{B.43}$$

Starting from Eq. (B.43), one can calculate the semiclassical static conductivity $\sigma_{\mu\nu}$ of a two-dimensional electron gas at zero temperature as

$$\sigma_{\mu\nu} = \frac{m^* e^2}{\pi\hbar^2} \int_0^\infty \left\langle v_\nu(0) v_\mu(t) \right\rangle^{(E_{\mathrm{F}})} dt, \tag{B.44}$$

where $\left\langle \left\{ \hat{v}_\nu(0), \hat{v}_\mu(t) \right\} \right\rangle_0^{(E_{\mathrm{F}})}$ has been replaced by the classical velocity autocorrelation function $\left\langle v_\nu(0) v_\mu(t) \right\rangle^{(E_{\mathrm{F}})} \overset{\mathrm{def}}{=} C_{\mu\nu}(t)$, which can be obtained numerically from simulated trajectories. The simplest way to take impurity scattering into account in such a calculation is to assume statistically independent scattering events that completely destroy any velocity correlation. If τ is the average time between two such scattering events, the probability that no scattering occurs in the time interval $[0, t]$ is $P(t) = \exp(-t/\tau)$, and the velocity autocorrelation function becomes $C_{\mu\nu}(t) = P(t)\check{C}_{\mu\nu}(t)$, where $\check{C}_{\mu\nu}(t)$ is calculated in the absence of impurity scattering [6].

Bibliography

[1] N. W. Ashcroft and D. N. Mermin. *Solid State Physics*, chapter 16. Harcourt College Publishers, Fort Worth, Texas, college edition, 1976.

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[5] KUBO [5] defines a *canonical momentum* $\langle \hat{A}; \hat{B} \rangle \overset{\mathrm{def}}{=} (1/\beta) \int_0^\beta \langle \exp(\lambda \hat{H}_0) \hat{A} \exp(-\lambda \hat{H}_0) \hat{B} \rangle_0^{(\beta)} d\lambda$. Then $(1/i\hbar) \langle [\hat{A}(0), \hat{B}(t)] \rangle_0^{(\beta)} = \beta \langle \dot{\hat{A}}(0); \hat{B}(t) \rangle$ and Eq. (B.39) is written $V\beta \int_0^\infty \langle \hat{J}_\nu(0); \hat{J}_\mu(t) \rangle \exp(-i\omega t)\, dt$. In the classical limit, both $\langle \hat{A}(0); \hat{B}(t) \rangle$ and $\langle \{ \hat{A}(0), \hat{B}(t) \} \rangle_0^{(\beta)}$ become the classical correlation function $\langle A(0) B(t) \rangle$.

[2] R. Kubo. Statistical-mechanical theory of irreversible processes. I. *Journal of the Physical Society of Japan*, 12(6):570–586, 1957.

[3] R. Kubo, M. Toda, and M. Hashitsume. *Statistical Physics II. Nonequilibrium Statistical Mechanics*, volume 31 of *Springer Series in Solid State Sciences*, chapter 4. Springer Verlag, Berlin, 1978.

[4] D. Cohen. Quantum pumping in closed systems, adiabatic transport, and the Kubo formula. *Physical Review B*, 2003.

[5] R. Kubo. The fluctuation–dissipation theorem. *Reports on Progress in Physics*, 29:255–284, 1966.

[6] R. Fleischmann, T. Geisel, and R. Ketzmerick. Magnetoresistance due to chaos and nonlinear resonances in lateral surface superlattices. *Physical Review Letters*, 68(9):1367–1370, March 1992.