# Theory of Electric Transport

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# 1 Linear response theory

## 1.1 Linear response and the Green function

Suppose the Hamilton operator of the system can be decomposed into the Hamilton operator of an unperturbed system, $H_0$ and the operator related to an, in general, time-dependent perturbation, $H'(t)$ :

$$H(t) = H_0 + H'(t) \ . \tag{1}$$

Using grand-canonical ensemble, the density operator of the unperturbed system can be written as

$$\varrho_0 = \frac{1}{\mathcal{Z}} \exp\left(-\beta \mathcal{H}_0\right) \ , \tag{2}$$

with $\beta = 1/k_B T$, $T$ the temperature, $k_B$ the Boltzmann constant, and

$$\mathcal{H}_0 = H_0 - \mu N \ , \tag{3}$$

where $\mu$ is the chemical potential, $N$ is the total (particle) number operator, and

$$\mathcal{Z} = Tr\left(\exp\left(-\beta \mathcal{H}_0\right)\right) \quad .$$

Within the Schrödinger picture the equation of motion for the density operator reads as

$$i\hbar \frac{\partial \varrho(t)}{\partial t} = \left[\mathcal{H}(t), \varrho(t)\right] \ , \tag{4}$$

where

$$\mathcal{H}(t) = H(t) - \mu N \ . \tag{5}$$

Clearly, in absence of the perturbation, $\varrho(t) = \varrho_0$. Partitioning, therefore, $\varrho(t)$ as

$$\varrho(t) = \varrho_0 + \varrho'(t) \ , \tag{6}$$

and making use that $[\mathcal{H}_0, \varrho_0] = 0$, we get *to first order in* $H'$,

$$i\hbar \frac{\partial \varrho'(t)}{\partial t} = \left[\mathcal{H}_0, \varrho'(t)\right] + \left[H'(t), \varrho_0\right] \ . \tag{7}$$

It is now worth to switch to the interaction (or Dirac) picture,

$$\varrho_D(t) = \varrho_0 + \varrho'_D(t) \ , \tag{8}$$

$$\varrho'_D(t) = \exp\left(\frac{i}{\hbar}\mathcal{H}_0 t\right) \varrho'(t) \exp\left(-\frac{i}{\hbar}\mathcal{H}_0 t\right) \ , \tag{9}$$

since

$$
\begin{aligned}
i\hbar\frac{\partial\varrho_D'(t)}{\partial t} &= [\varrho_D'(t), \mathcal{H}_0] + \underbrace{\exp\left(\frac{i}{\hbar}\mathcal{H}_0 t\right) i\hbar\frac{\partial\varrho'(t)}{\partial t}\exp\left(-\frac{i}{\hbar}\mathcal{H}_0 t\right)}_{[\mathcal{H}_0, \varrho_D'(t)] + [H_D'(t), \varrho_0]} \\
&= [H_D'(t), \varrho_0] \ . \qquad (10)
\end{aligned}
$$

The solution of the above equation with the boundary condition $\varrho_D'(t) \underset{t\to-\infty}{\longrightarrow} 0$ can be given as

$$
\varrho_D'(t) = -\frac{i}{\hbar}\int_{-\infty}^{t} dt' \ [H_D'(t'), \varrho_0] \ , \qquad (11)
$$

thus, returning back to the Schrödinger picture, the density operator can be approximated to first order as

$$
\varrho(t) \approx \varrho_0 - \frac{i}{\hbar}\int_{-\infty}^{t} dt' \ \exp\left(-\frac{i}{\hbar}\mathcal{H}_0 t\right)[H_D'(t'), \varrho_0]\exp\left(\frac{i}{\hbar}\mathcal{H}_0 t\right) \ . \qquad (12)
$$

Considering the time evolution of a physical observable, say $A(t)$, associated with a Hermitean operator, $A$ one gets

$$
\begin{aligned}
A(t) &= A_0 - \frac{i}{\hbar}\int_{-\infty}^{t} dt' \, Tr\left\{\exp\left(-\frac{i}{\hbar}\mathcal{H}_0 t\right)[H_D'(t'), \varrho_0]\exp\left(\frac{i}{\hbar}\mathcal{H}_0 t\right) A\right\} \\
&= A_0 - \frac{i}{\hbar}\int_{-\infty}^{t} dt' \, Tr\left\{[H_D'(t'), \varrho_0] \ A_D(t)\right\} \ , \qquad (13)
\end{aligned}
$$

where $A_0 = Tr\{\varrho_0 A\}$ and the Dirac representation of operator $A$,

$$
A_D(t) = \exp\left(\frac{i}{\hbar}\mathcal{H}_0 t\right) A \exp\left(-\frac{i}{\hbar}\mathcal{H}_0 t\right) \ , \qquad (14)
$$

is used. Applying the identity,

$$
Tr\{[A,B]\,C\} = Tr\{ABC - BAC\} = Tr\{BCA - BAC\} = Tr\{B\,[C,A]\} \ ,
$$

we get

$$
\delta A(t) = -\frac{i}{\hbar}\int_{-\infty}^{t} dt' \, Tr\{\varrho_0\,[A_D(t), H_D'(t')]\} \ , \qquad (15)
$$

by defining $\delta A(t) \equiv A(t) - A_0$. In general, the perturbation $H'(t)$ has the form,

$$
H'(t) = -B\,F(t) \ , \qquad (16)
$$

where $B$ is a Hermitean operator and $F(t)$ is a complex function (classical field). In that case, Eq. (15) transforms into

$$
\delta A(t) = -\frac{i}{\hbar}\int_{-\infty}^{t} dt' \, F(t') \ Tr\{\varrho_0\,[A_D(t), B_D(t')]\} \ , \qquad (17)
$$

or written in terms of the *retarded Green function*,

$$G^{ret}_{AB}(t,t') = -i\,\Theta(t-t')\;Tr\left\{\varrho_0\left[A_D(t)\,,B_D(t')\right]\right\}\;, \tag{18}$$

$$\delta A(t) = \frac{1}{\hbar}\int_{-\infty}^{\infty} dt'\,F(t')\;G^{ret}_{AB}(t,t')\;. \tag{19}$$

It should be noted that since the time-evolution in the Dirac picture is governed by $H_0$, the operators $A_D(t)$ and $B_D(t')$ are equivalent with the corresponding Heisenberg-operators related to the unperturbed system, as most commonly used in the definition of the Green function, Eq. (18). Supposing that the operators $A$ and $B$ do not explicitly depend on time, $G^{ret}_{AB}(t,t')$ will be a function of $t-t'$. Therefore, the Fourier coefficients of $\delta A(t)$ can be written as

$$\delta A(\omega) = \frac{1}{\hbar}F(\omega)\;G^{ret}_{AB}(\omega)\;, \tag{20}$$

where

$$X(\omega) = \int_{-\infty}^{\infty} dt\,X(t)\exp(i\omega t) \tag{21}$$

and

$$X(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega\,X(\omega)\exp(-i\omega t)\;, \tag{22}$$

for any time-dependent quantity, $X(t)$. Care has, however, to be taken since $G^{ret}_{AB}(\varpi)$ is analytical in the upper complex semiplane (retarded sheet) only. As a consequence, for a real argument $\omega$, the limit $\varpi \to \omega + i0$ has to be considered! The complex admittance, $\chi_{AB}(\omega)$ defined as

$$\delta A(\omega) = F(\omega)\;\chi_{AB}(\omega)\;, \tag{23}$$

can then be expressed as

$$\chi_{AB}(\omega) = \frac{1}{\hbar}\,G^{ret}_{AB}(\omega+i0) = -\frac{i}{\hbar}\int_0^{\infty} dt\;\exp\left(i(\omega+i0)\,t\right)\;Tr\left\{\varrho_0\left[A(t)\,,B(0)\right]\right\}\;. \tag{24}$$

The appearance of the side-limit, $\omega+i0$, in $\chi_{AB}(\omega)$ is usually termed as the *adiabatic switching* of the perturbation as it corresponds to a time-dependent classical field,

$$F'(t) = \lim_{s\to 0} F(t)\,e^{st}\;. \tag{25}$$

## 1.2 The Kubo formula

Let's come back to the expression (13),

$$\delta A(t) = -\frac{i}{\hbar}\int_{-\infty}^{t} dt'\,Tr\left\{\left[H'_H(t')\,,\varrho_0\right]\;A_H(t)\right\}\;, \tag{26}$$

where the operators are taken in the Heisenberg picture with respect to the unperturbed system.

*Kubo's identity:*

$$\frac{i}{\hbar}\left[X_H\left(t\right),\varrho\right]=\varrho\int_0^\beta d\lambda\,\dot{X}_H\left(t-i\lambda\hbar\right)\ , \tag{27}$$

where

$$\varrho=\frac{\exp\left(-\beta H\right)}{Tr\left\{\exp\left(-\beta H\right)\right\}}\ ,\qquad X_H\left(t\right)=\exp\left(\frac{i}{\hbar}Ht\right)\,X\left(t\right)\exp\left(-\frac{i}{\hbar}Ht\right)\ ,$$
$$\text{and}\quad \dot{X}_H\left(t\right)=-\frac{i}{\hbar}\left[X_H\left(t\right),H\right]\ .$$

*Proof*:

$$\begin{aligned}
&\varrho\int_0^\beta d\lambda\,\dot{X}_H\left(t-i\lambda\hbar\right)=\\
&=-\frac{i}{\hbar}\varrho\int_0^\beta d\lambda\,\left[\exp\left(\lambda H\right)\,X_H\left(t\right)\exp\left(-\lambda H\right),H\right]\\
&=\frac{i}{\hbar}\varrho\int_0^\beta d\lambda\,\frac{d}{d\lambda}\left[\exp\left(\lambda H\right)\,X_H\left(t\right)\exp\left(-\lambda H\right)\right]\\
&=\frac{i}{\hbar}(\underbrace{\varrho\exp\left(\beta H\right)\,X_H\left(t\right)\exp\left(-\beta H\right)}_{X_H(t)\,\varrho}-\rho A_H\left(t\right))\\
&=\frac{i}{\hbar}\left[X_H\left(t\right),\varrho\right]\ .
\end{aligned}$$

Employing Kubo's identity (27) in Eq. (26) yields

$$\begin{aligned}
\delta A\left(t\right)&=-\int_{-\infty}^t dt'\int_0^\beta d\lambda\,Tr\left\{\varrho_0\,\dot{H}'_H\left(t'-i\lambda\hbar\right)\,A_H\left(t\right)\right\}\\
&=-\int_{-\infty}^t dt'\int_0^\beta d\lambda\,Tr\left\{\varrho_0\,\dot{H}'\left(t'\right)\,A_H\left(t-t'+i\lambda\hbar\right)\right\}\ ,
\end{aligned} \tag{28}$$

since

$$\begin{aligned}
&Tr\left\{\varrho_0\,\dot{H}'_H\left(t'-i\lambda\hbar\right)\,A_H\left(t\right)\right\}=\\
&=Tr\left\{\varrho_0\,\exp\left(\frac{i}{\hbar}\left(t'-i\lambda\hbar\right)\mathcal{H}_0\right)\dot{H}'\left(t'\right)\exp\left(-\frac{i}{\hbar}\left(t'-i\lambda\hbar\right)\mathcal{H}_0\right)\,A_H\left(t\right)\right\}\\
&=Tr\left\{\varrho_0\,\dot{H}'\left(t'\right)\,\exp\left(-\frac{i}{\hbar}\left(t'-i\lambda\hbar\right)\mathcal{H}_0\right)A_H(t)\exp\left(\frac{i}{\hbar}\left(t'-i\lambda\hbar\right)\mathcal{H}_0\right)\right\}\\
&=Tr\left\{\varrho_0\,\dot{H}'\left(t'\right)\,A_H\left(t-t'+i\lambda\hbar\right)\right\}\ .
\end{aligned}$$

## 2 The electric conductivity tensor

### 2.1 The current-current correlation function

In case of electric transport a time dependent external electric field is applied to a solid. Obviously, this induces currents, which in turn creates internal electric fields. Let us assume that the total electric field, $\vec{E}(\vec{r},t)$ is related to the perturbation through a scalar potential, $\phi(\vec{r},t)$ ( $\vec{E}(\vec{r},t) = -\vec{\nabla}\phi(\vec{r},t)$ )

$$H'(t) = \int d^3r\, \rho(\vec{r})\, \phi(\vec{r},t) \ , \tag{29}$$

where $\rho(\vec{r}) = e\, \psi(\vec{r})^+ \psi(\vec{r})$ is the operator of the charge density, with $\psi(\vec{r})$ being the field operator and $e$ the charge of the electron. (A derivation of the conductivity tensor is possible also assuming a vectorpotential, $\vec{A}(\vec{r},t)$, related to the electric field by $\vec{E}(\vec{r},t) = -\frac{1}{c}\frac{d\vec{A}(\vec{r},t)}{dt}$, which in turn leads to an identical result as derived here.) The time-derivative of $H'_H(t)$ can be calculated as follows,

$$\begin{aligned} \dot{H}'(t) &= \int d^3r\, \underbrace{\frac{1}{i\hbar}\left[\mathcal{H}_0, \rho(\vec{r})\right]}_{\frac{\partial \rho_H(\vec{r},t)}{\partial t}|_{t=0}} \phi(\vec{r},t) = -\int d^3r\, \vec{\nabla}\vec{J}(\vec{r})\ \phi(\vec{r},t) \\ &= \int d^3r\ \vec{J}(\vec{r})\ \vec{\nabla}\phi(\vec{r},t) = -\int d^3r\ \vec{J}(\vec{r})\ \vec{E}(\vec{r},t) \ , \end{aligned} \tag{30}$$

with the current-density operator,

$$\vec{J}(\vec{r}) = \begin{cases} \frac{e\hbar}{2mi}\, \psi(\vec{r})^+ \left(\overrightarrow{\nabla} - \overleftarrow{\nabla}\right) \psi(\vec{r}) & \text{in non-relativistic case} \\ \\ ec\, \psi(\vec{r})^+\ \vec{\alpha}\, \psi(\vec{r}) & \text{in relativistic case} \end{cases} \ , \tag{31}$$

and the Dirac matrices, $\vec{\alpha}$. Note that in Eq. (30) we made use of the continuity equation and we assumed periodic boundary conditions at the surface of the solid, therefore, when using Gauss' integration theorem the corresponding surface term vanished. Making use of Eqs. (28) and (30) the $\mu$th component of the current can be written as

$$J_\mu(\vec{r},t) = \sum_\nu \int d^3r' \int_{-\infty}^{\infty} dt'\ \sigma_{\mu\nu}(\vec{r},\vec{r}\,';t,t')\, E_\nu(\vec{r}\,',t') \ , \tag{32}$$

where the space-time correlation function is given by

$$\sigma_{\mu\nu}(\vec{r},\vec{r}\,';t,t') = \Theta(t-t') \int_0^\beta d\lambda\, Tr\left\{\varrho_0\, J_\nu(\vec{r},0)\ J_\mu(\vec{r}\,',t-t'+i\lambda\hbar)\right\} \ , \tag{33}$$

expressing the linear response of the current at $(\vec{r},t)$ in direction $\mu$ to the local electric field at $(\vec{r}\,',t')$ applied in direction $\nu$. Note that in the above equation the current-density operators are assumed to be Heisenberg operators.

As before, we look for the response of a Fourier component of the electric field,

$$\vec{E}(\vec{r},t) = \frac{1}{2\pi V}\,\vec{E}\,(\vec{q},\omega)\ \exp\left(i\vec{q}\,\vec{r} - i\varpi t\right)\ , \tag{34}$$

$$\left(\ \vec{E}\,(\vec{q},\omega) = \int_{-\infty}^{\infty} dt \int d^3r\,\vec{E}(\vec{r},t)\exp\left(-i\vec{q}\,\vec{r} + i\varpi t\right)\ \right)$$

where $\varpi = \omega + i0$ and $V$ is the volume of the system. While $\sigma_{\mu\nu}(\vec{r},\vec{r}\,';t,t')$ trivially depends on $t - t'$ (see. Eq. (33)), in general, it is a function of independent space variables, $\vec{r}$ and $\vec{r}\,'$. In cases, when the measured current is an average of the local current defined in (32) over a big region (many cells) of the solids, the assumption that $\sigma_{\mu\nu}(\vec{r},\vec{r}\,';t,t')$ is homogeneous in space, i.e., $\sigma_{\mu\nu}(\vec{r},\vec{r}\,';t-t') = \sigma_{\mu\nu}(\vec{r}-\vec{r}\,';t-t')$, can be made, which facilitates a direct Fourier transformation of Eq. (32). Usually this happens when $\vec{q}$ is small, that means when *long-wavelength excitations* are studied. The $(\vec{q},\omega)$ component of the current per unit volume,

$$J_\mu(\vec{q},\omega) = \frac{1}{V}\int_{-\infty}^{\infty} dt \int d^3r\ J_\mu(\vec{r},t)\exp\left(-i\vec{q}\,\vec{r} + i\varpi t\right) \tag{35}$$

can then be determined from Eqs. (32) and (33),

$$J_\mu(\vec{q},\omega) = \sum_\nu \sigma_{\mu\nu}(\vec{q},\omega)\,E_\nu(\vec{q},\omega)\ , \tag{36}$$

with the wave–vector and frequency dependent *conductivity tensor* $\sigma_{\mu\nu}(\vec{q},\omega)$

$$\sigma_{\mu\nu}(\vec{q},\omega) = \frac{1}{V}\int_0^{\infty} dt\ \exp\left(i\varpi t\right)\int_0^{\beta} d\lambda\ Tr\left\{\varrho_0 J_\nu\left(-\vec{q},0\right) J_\mu\left(\vec{q},t+i\hbar\lambda\right)\right\}\ , \tag{37}$$

with

$$J_\mu\left(\vec{q},t\right) = \int d^3r\ J_\mu\left(\vec{r}\,',t\right)\exp\left(-i\vec{q}\,\vec{r}\right)\ . \tag{38}$$

After some algebra,

$$\begin{aligned}
&\int_0^{\beta} d\lambda\ Tr\left\{\varrho_0\ J_\nu\left(-\vec{q},0\right)\ J_\mu\left(\vec{q},t+i\hbar\lambda\right)\right\}\\
&= \int_0^{\beta} d\lambda\ \frac{1}{\mathcal{Z}}Tr\left\{\exp\left(-\beta\mathcal{H}_0\right)\ J_\nu\left(-\vec{q},0\right)\ \exp\left(-\lambda\mathcal{H}_0\right)\ J_\mu\left(\vec{q},t\right)\exp\left(\lambda\mathcal{H}_0\right)\right\}\\
&= \int_0^{\beta} d\lambda\ \frac{1}{\mathcal{Z}}Tr\left\{\exp\left(-\lambda\mathcal{H}_0\right)\ J_\mu\left(\vec{q},t\right)\exp\left(\left(\lambda-\beta\right)\mathcal{H}_0\right)\ J_\nu\left(-\vec{q},0\right)\right\}\\
&= \int_0^{\beta} d\lambda\ Tr\left\{\varrho_0\ \exp\left(\left(\beta-\lambda\right)\mathcal{H}_0\right)\ J_\mu\left(\vec{q},t\right)\exp\left(\left(\lambda-\beta\right)\mathcal{H}_0\right)\ J_\nu\left(-\vec{q},0\right)\right\}\\
&= \int_0^{\beta} d\lambda\ Tr\left\{\varrho_0\ \exp\left(\lambda\mathcal{H}_0\right)\ J_\mu\left(\vec{q},t\right)\exp\left(-\lambda\mathcal{H}_0\right)\ J_\nu\left(-\vec{q},0\right)\right\}\\
&= \int_0^{\beta} d\lambda\ Tr\left\{\varrho_0\ J_\mu\left(\vec{q},t-i\hbar\lambda\right)\ J_\nu\left(-\vec{q},0\right)\right\}
\end{aligned}$$

and contour integration tricks,

$$\begin{aligned}
&\int_0^\beta d\lambda \; Tr\left\{\varrho_0 J_\mu\left(\vec{q}, t - i\hbar\lambda\right) J_\nu\left(-\vec{q}, 0\right)\right\} \\
&= \frac{i}{\hbar}\int_t^{t-i\hbar\beta} d\tau \; Tr\left\{\varrho_0 J_\mu\left(\vec{q}, \tau\right) J_\nu\left(-\vec{q}, 0\right)\right\} \\
&= \frac{i}{\hbar}\int_t^{\infty} dt' \; Tr\left\{\varrho_0 \;\left(J_\mu\left(\vec{q}, t'\right) J_\nu\left(-\vec{q}, 0\right) - J_\mu\left(\vec{q}, t' - i\hbar\beta\right) J_\nu\left(-\vec{q}, 0\right)\right)\right\} \\
&= \frac{i}{\hbar}\int_t^{\infty} dt' \; Tr\left\{\varrho_0 \;\left(J_\mu\left(\vec{q}, t'\right) J_\nu\left(-\vec{q}, 0\right) - J_\nu\left(-\vec{q}, 0\right) J_\mu\left(\vec{q}, t'\right)\right)\right\} \\
&= \frac{i}{\hbar}\int_t^{\infty} dt' \; Tr\left\{\varrho_0 \;\left[J_\mu\left(\vec{q}, t'\right), J_\nu\left(-\vec{q}, 0\right)\right]\right\} \quad ,
\end{aligned}$$

where we assumed that the integrand is analytical, we arrive at

$$\sigma_{\mu\nu}(\vec{q}, \omega) = \frac{i}{\hbar V}\int_0^\infty dt \; \exp\left(i\varpi t\right)\int_t^\infty dt' \; Tr\left\{\varrho_0 \;\left[J_\mu\left(\vec{q}, t'\right), J_\nu\left(-\vec{q}, 0\right)\right]\right\} \; . \tag{39}$$

Integration by part yields,

$$\begin{aligned}
&\frac{1}{\hbar V\varpi}\int_0^\infty dt \; \frac{d\exp\left(i\varpi t\right)}{dt}\int_t^\infty dt' \; Tr\left\{\varrho_0 \;\left[J_\mu\left(\vec{q}, t'\right), J_\nu\left(-\vec{q}, 0\right)\right]\right\} = \\
&\frac{1}{\hbar V\varpi}\left(\left[\exp\left(i\varpi t\right)\int_t^\infty dt' \; Tr\left\{\varrho_0 \;\left[J_\mu\left(\vec{q}, t'\right), J_\nu\left(-\vec{q}, 0\right)\right]\right\}\right]_0^\infty \right.\\
&\qquad \left. + \int_0^\infty dt \; \exp\left(i\varpi t\right) \; Tr\left\{\varrho_0 \;\left[J_\mu\left(\vec{q}, t\right), J_\nu\left(-\vec{q}, 0\right)\right]\right\}\right) = \\
&\frac{1}{\hbar V\varpi}\left(\int_0^\infty dt \; \exp\left(i\varpi t\right) \; Tr\left\{\varrho_0 \;\left[J_\mu\left(\vec{q}, t\right), J_\nu\left(-\vec{q}, 0\right)\right]\right\}\right.\\
&\qquad \left. - \int_0^\infty dt' \; Tr\left\{\varrho_0 \;\left[J_\mu\left(\vec{q}, t'\right), J_\nu\left(-\vec{q}, 0\right)\right]\right\}\right) \; .
\end{aligned}$$

By introducing the current-current correlation function,

$$\Sigma_{\mu\nu}(\vec{q}, \varpi) = \frac{1}{\hbar V}\int_0^\infty dt \; \exp\left(i\varpi t\right) \; Tr\left\{\varrho_0 \;\left[J_\mu\left(\vec{q}, t\right), J_\nu\left(-\vec{q}, 0\right)\right]\right\} \; , \tag{40}$$

the conductivity tensor can be expressed as

$$\sigma_{\mu\nu}(\vec{q}, \omega) = \frac{\Sigma_{\mu\nu}(\vec{q}, \varpi) - \Sigma_{\mu\nu}(\vec{q}, 0)}{\varpi} \; . \tag{41}$$

For a homogeneous system with carrier density, $n$ and mass of the carriers, $m$,

$$-\frac{\Sigma_{\mu\nu}(\vec{q}, 0)}{\varpi} = i\frac{ne^2}{m\varpi}\delta_{\mu\nu} \; , \tag{42}$$

i.e., the phenomenological Drude term for non-interacting particles. It is furthermore clear, that the static, i.e., $\omega \to 0$ (and $\vec{q} \to 0$), limit has to be performed as

$$\begin{aligned}
\sigma_{\mu\nu}(\vec{q} = 0, \omega = 0) &= \lim_{s\to+0}\frac{\Sigma_{\mu\nu}(\vec{q} = 0, is) - \Sigma_{\mu\nu}(\vec{q} = 0, 0)}{is} \\
&= \left.\frac{d\,\Sigma_{\mu\nu}(\vec{q} = 0, \varpi)}{d\varpi}\right|_{\varpi=0} \; .
\end{aligned} \tag{43}$$

We shall derive more specific expressions for a system of non-interacting particles.

## 2.2 Kubo formula for independent particles

Skipping the quite straigthforward but lengthy derivation, we can state that formulas (37), (39) or (40-41) apply also for a system of independent particles (fermions), when the corresponding one-particle operators and the Fermi-Dirac distribution,

$$\rho_0 \equiv f(H_0) = \frac{1}{e^{\beta(H_0-\mu)}+1} \tag{44}$$

is used. Working in the basis of eigenfuctions of $H_0$,

$$H_0 \left|n\right\rangle = \varepsilon_n \left|n\right\rangle \ , \quad \langle\, m \,|\, n \,\rangle = \delta_{nm} \ , \quad \sum_n |\, n \,\rangle\langle\, n \,| = I \ ,$$

the thermal average of the current–current commutator can be written as

$$\begin{aligned} &Tr\left\{\varrho_0 \ \left[J_\mu\left(\vec{q},t'\right), J_\nu\left(-\vec{q},0\right)\right]\right\} = \\ &= \sum_{n,m} \ \left[f(\varepsilon_n)-f(\varepsilon_m)\right] \ \exp\left(\frac{i}{\hbar}(\varepsilon_n-\varepsilon_m)t'\right) \ J_\mu^{nm}\left(\vec{q}\right) J_\nu^{mn}\left(-\vec{q}\right) \ , \end{aligned} \tag{45}$$

with

$$J_\mu^{nm}\left(\vec{q}\right) \equiv \left\langle n\right| J_\mu\left(\vec{q}\right)\left|m\right\rangle \quad \text{and} \quad J_\nu^{mn}\left(-\vec{q}\right) \equiv \left\langle m\right| J_\nu\left(-\vec{q}\right)\left|n\right\rangle \ . \tag{46}$$

Namely,

$$\begin{aligned} &Tr\left\{\varrho_0 \ \left[J_\mu\left(\vec{q},t'\right), J_\nu\left(-\vec{q},0\right)\right]\right\} = \\ &= \sum_{n,m,p} \langle\, n \,|\, f(H_0) |\, p \,\rangle\langle\, p \,|\, e^{\frac{i}{\hbar}H_0 t'} J_\mu\left(\vec{q},t'\right) e^{-\frac{i}{\hbar}H_0 t'} |\, m \,\rangle \,\langle\, m \,| J_\nu\left(-\vec{q}\right) |\, n \,\rangle \\ &- \sum_{m,n,p} \langle\, m \,|\, f(H_0) |\, p \,\rangle \,\langle\, p \,| J_\nu\left(-\vec{q}\right) |\, n \,\rangle\langle\, n \,|\, e^{\frac{i}{\hbar}H_0 t'} J_\mu\left(\vec{q},t'\right) e^{-\frac{i}{\hbar}H_0 t'} |\, m \,\rangle \ , \end{aligned}$$

and

$$\left\langle n\right| f(H_0) \left|p\right\rangle = f(\varepsilon_n)\delta_{pn}$$

$$\Downarrow$$

$$\begin{aligned} &Tr\left\{\varrho_0 \ \left[J_\mu\left(\vec{q},t'\right), J_\nu\left(-\vec{q},0\right)\right]\right\} = \\ &= \sum_{n,m} f(\varepsilon_n)\, e^{\frac{i}{\hbar}\varepsilon_n t'} J_\mu^{nm}\left(\vec{q}\right) e^{-\frac{i}{\hbar}\varepsilon_m t'} J_\nu^{mn}\left(-\vec{q}\right) \\ &- \sum_{m,n} f(\varepsilon_m)\, J_\nu^{mn}\left(-\vec{q}\right) e^{\frac{i}{\hbar}\varepsilon_n t'} J_\mu^{nm}\left(\vec{q}\right) e^{-\frac{i}{\hbar}\varepsilon_m t'} \ . \end{aligned}$$

Substituting Eq. (45) into Eq. (40) yields

$$\begin{aligned} \Sigma_{\mu\nu}(\vec{q},\omega) = &\frac{1}{\hbar V} \sum_{n,m} \ \left[f(\varepsilon_n)-f(\varepsilon_m)\right] \ J_\mu^{nm}\left(\vec{q}\right) J_\nu^{mn}\left(-\vec{q}\right) \\ &\cdot \int_0^\infty dt \ \exp\left(\frac{i}{\hbar}(\varepsilon_n-\varepsilon_m+\hbar\varpi)t\right) \ . \end{aligned} \tag{47}$$

The integral on the right–hand side with respect to $t$ is just the Laplace transform of the identity,

$$\int_0^\infty dt \ \exp\left(\left[-s + \frac{i}{\hbar}(\varepsilon_n - \varepsilon_m + \hbar\omega)\right] t\right) \underset{(s>0)}{=} \\ -\frac{\exp\left(\left[-s + \frac{i}{\hbar}(\varepsilon_n - \varepsilon_m + \hbar\omega)\right] t\right)}{-s + \frac{i}{\hbar}(\varepsilon_n - \varepsilon_m + \hbar\omega)} \ , \tag{48}$$

therefore, Eq. (47) can be transformed to

$$\Sigma_{\mu\nu}(\vec{q},\omega) = \frac{i}{V} \sum_{n,m} \frac{f(\varepsilon_n) - f(\varepsilon_m)}{\varepsilon_n - \varepsilon_m + \hbar\varpi} \ J_\mu^{nm}(\vec{q}) \, J_\nu^{mn}(-\vec{q}) \quad , \tag{49}$$

which together with Eq. (39) provides a numerically tractable tool to calculate the conductivity tensor.

It is worth to mention that since

$$\frac{1}{\varepsilon_n - \varepsilon_m + \hbar\varpi} - \frac{1}{\varepsilon_n - \varepsilon_m} = -\frac{\hbar\varpi}{(\varepsilon_n - \varepsilon_m)(\varepsilon_n - \varepsilon_m + \hbar\varpi)} \ ,$$

$\sigma_{\mu\nu}(\vec{q};\omega)$ can be written into the compact form,

$$\sigma_{\mu\nu}(\vec{q};\omega) = \frac{\hbar}{iV} \sum_{n,m} \frac{f(\varepsilon_n) - f(\varepsilon_m)}{\varepsilon_n - \varepsilon_m} \ \frac{J_\mu^{nm}(\vec{q}) \, J_\nu^{mn}(-\vec{q})}{\varepsilon_n - \varepsilon_m + \hbar\varpi} \ . \tag{50}$$

It should also be noted that in calculations of optical spectra a finite (positive) value of $\delta$ is considered in order to account for finite life-time effects. It is easy to show, that this is indeed equivalent by folding the spectrum with a Lorentzian of half-width $\delta$. Therefore, we often speak about the *complex conductivity tensor*, $\sigma_{\mu\nu}(\vec{q},\varpi)$.

## 2.3 Contour integration technique

As what follows we evaluate $\Sigma_{\mu\nu}(\vec{q},\varpi)$ by using a contour integration technique, keeping in mind that we have a finite imaginary part of the denominator in Eq. (49). Consider a pair of eigenvalues, $\epsilon_n$ and $\epsilon_m$. For a suitable contour $\Gamma_1$ in the complex energy plane (see Fig. 1) the residue theorem implies

$$\oint_{\Gamma_1} dz \, \frac{f(z)}{(z-\epsilon_n)(z-\epsilon_m+\hbar\omega+i\delta)} = -2\pi i \frac{f(\epsilon_n)}{\epsilon_n - \epsilon_m + \hbar\omega + i\delta} \\ +2i\delta_T \sum_{k=-N_2+1}^{N_1} \frac{1}{(z_k-\epsilon_n)(z_k-\epsilon_m+\hbar\omega+i\delta)} \quad , \tag{51}$$

where the $z_k = \epsilon_F + i(2k-1)\delta_T$ ($\epsilon_F$ is the Fermi energy, $k_B$ the Boltzmann constant, $T$ the temperature and $\delta_T \equiv \pi k_B T$) are the (fermionic) Matsubara-poles. In Eq. (51) it was supposed that $N_1$ and $N_2$ Matsubara-poles in the upper and lower semi-plane lie within the contour $\Gamma_1$, respectively, i.e.,

$$(2N_1 - 1)\delta_T < \delta_1 < (2N_1 + 1)\delta_T \ , \tag{52}$$

$$(2N_2 - 1)\delta_T < \delta_2 < (2N_2 + 1)\delta_T \ . \tag{53}$$

Eq. (51) can be rearranged as

$$i\frac{f(\epsilon_n)}{\epsilon_n - \epsilon_m + \hbar\omega + i\delta} = -\frac{1}{2\pi}\oint_{\Gamma_1} dz\, \frac{f(z)}{(z-\epsilon_n)(z-\epsilon_m+\hbar\omega+i\delta)} + i\frac{\delta_T}{\pi}\sum_{k=-N_2+1}^{N_1} \frac{1}{(z_k-\epsilon_n)(z_k-\epsilon_m+\hbar\omega+i\delta)} \quad . \tag{54}$$

Similarly, by choosing a contour $\Gamma_2$ (in fact, $\Gamma_1$ mirrored to the real axis, see figure) the following expression,

$$-i\frac{f(\epsilon_m)}{\hbar\omega + \epsilon_n - \epsilon_m + i\delta} = \frac{1}{2\pi}\oint_{\Gamma_2} dz\, \frac{f(z)}{(z-\epsilon_m)(z-\epsilon_n-\hbar\omega-i\delta)} + i\frac{\delta_T}{\pi}\sum_{k=-N_1+1}^{N_2} \frac{1}{(z_k-\epsilon_m)(z_k-\epsilon_n-\hbar\omega-i\delta)} \ , \tag{55}$$

can be derived.

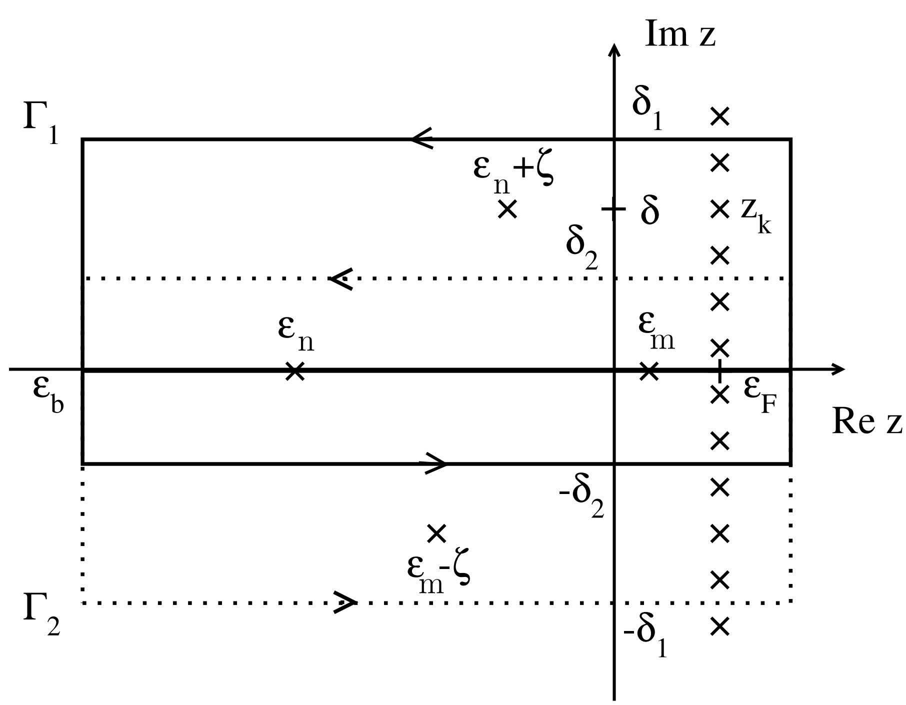


Figure 1: Schematic view of contours $\Gamma_1$ and $\Gamma_2$ ($\zeta = \hbar\omega + i\delta$).

Inserting Eqs. (54) and (55) into Eq. (49) and by extending the contours to cross the real axis at $\infty$ and $-\infty$, $\Sigma_{\mu\nu}(\varpi)$ can be expressed as

$$\begin{aligned}\Sigma_{\mu\nu}(\vec{q},\varpi) = &-\frac{1}{2\pi V}\left\{\oint_{\Gamma_1} dz\, f(z) \sum_{m,n} \frac{J_\mu^{nm}(\vec{q})\, J_\nu^{mn}(-\vec{q})}{(z-\epsilon_n)(z-\epsilon_m+\hbar\omega+i\delta)} - \right.\\ &\left.\oint_{\Gamma_2} dz\, f(z) \sum_{m,n} \frac{J_\mu^{nm}(\vec{q})\, J_\nu^{mn}(-\vec{q})}{(z-\epsilon_m)(z-\epsilon_n-\hbar\omega-i\delta)}\right\}\\ &+ i\frac{\delta_T}{\pi V}\left\{\sum_{k=-N_2+1}^{N_1} \sum_{m,n} \frac{J_\mu^{nm}(\vec{q})\, J_\nu^{mn}(-\vec{q})}{(z_k-\epsilon_n)(z_k-\epsilon_m+\hbar\omega+i\delta)} + \right.\\ &\left.\sum_{k=-N_1+1}^{N_2} \sum_{m,n} \frac{J_\mu^{nm}(\vec{q})\, J_\nu^{mn}(-\vec{q})}{(z_k-\epsilon_m)(z_k-\epsilon_n-\hbar\omega-i\delta)}\right\} \quad .\end{aligned} \tag{56}$$

It is now straightforward to rewrite Eq. (56) in terms of the resolvent,

$$G(z) = \sum_n \frac{|\, n\,\rangle\langle\, n\,|}{z-\epsilon_n} \;, \tag{57}$$

such that

$$\begin{aligned}\Sigma_{\mu\nu}(\vec{q},\varpi) = &-\frac{1}{2\pi V}\left\{\oint_{\Gamma_1} dz\, f(z)\, Tr\left[J_\mu(\vec{q})\; G(z+\hbar\omega+i\delta)\, J_\nu(-\vec{q})\; G(z)\right] - \right.\\ &\left.\oint_{\Gamma_2} dz\, f(z)\, Tr\left[J_\mu(\vec{q})\; G(z) J_\nu(-\vec{q})\; G(z-\hbar\omega-i\delta)\right]\right\}\\ &+ i\frac{\delta_T}{\pi V}\left\{\sum_{k=-N_2+1}^{N_1} Tr\left[J_\mu(\vec{q})\; G(z_k+\hbar\omega+i\delta)\, J_\nu(-\vec{q})\; G(z_k)\right] + \right.\\ &\left.\sum_{k=-N_1+1}^{N_2} Tr\left[J_\mu(\vec{q})\; G(z_k)\, J_\nu(-\vec{q})\; G(z_k-\hbar\omega-i\delta)\right]\right\} \;.\end{aligned} \tag{58}$$

By using the quantity,

$$\widetilde{\Sigma}_{\mu\nu}(\vec{q};z_1,z_2) = -\frac{1}{2\pi V} Tr\left[J_\mu(\vec{q})\; G(z_1)\, J_\nu(-\vec{q})\, G(z_2)\right] \;, \tag{59}$$

for which the following symmetry relations apply,

$$\widetilde{\Sigma}_{\nu\mu}(-\vec{q};z_2,z_1) = \widetilde{\Sigma}_{\mu\nu}(\vec{q};z_1,z_2) \;, \tag{60}$$

$$\widetilde{\Sigma}_{\mu\nu}(\vec{q};z_1^*,z_2^*) = \widetilde{\Sigma}_{\nu\mu}(\vec{q};z_1,z_2)^* = \widetilde{\Sigma}_{\mu\nu}(-\vec{q};z_2,z_1)^*, \tag{61}$$

$\Sigma_{\mu\nu}(\vec{q};\varpi)$ can be written as

$$
\begin{aligned}
\Sigma_{\mu\nu}(\vec{q},\varpi) = & \oint_{\Gamma_1} dz\, f(z)\, \widetilde{\Sigma}_{\mu\nu}(\vec{q}; z+\hbar\omega+i\delta, z) \\
& - \oint_{\Gamma_2} dz\, f(z)\, \widetilde{\Sigma}_{\mu\nu}(\vec{q}; z, z-\hbar\omega-i\delta) \\
& -2i\delta_T \left\{ \sum_{k=-N_2+1}^{N_1} \widetilde{\Sigma}_{\mu\nu}(\vec{q}; z_k+\hbar\omega+i\delta, z_k) \right. \\
& \left. + \sum_{k=-N_1+1}^{N_2} \widetilde{\Sigma}_{\mu\nu}(\vec{q}; z_k, z_k-\hbar\omega-i\delta) \right\} ,
\end{aligned}
\tag{62}
$$

which because of the reflection symmetry for the contours $\Gamma_1$ and $\Gamma_2$ (see figures) and the relations in Eqs. (60-61) can be transformed to

$$
\begin{aligned}
\Sigma_{\mu\nu}(\vec{q},\varpi) = & \oint_{\Gamma_1} dz\, f(z)\, \widetilde{\Sigma}_{\mu\nu}(\vec{q}; z+\hbar\omega+i\delta, z) \\
& - \left( \oint_{\Gamma_1} dz\, f(z)\, \widetilde{\Sigma}_{\mu\nu}(-\vec{q}; z-\hbar\omega+i\delta, z) \right)^* \\
& -2i\delta_T \sum_{k=-N_2+1}^{N_1} \left\{ \widetilde{\Sigma}_{\mu\nu}(\vec{q}; z_k+\hbar\omega+i\delta, z_k) \right. \\
& \left. + \widetilde{\Sigma}_{\mu\nu}(-\vec{q}; z_k-\hbar\omega+i\delta, z_k)^* \right\} .
\end{aligned}
\tag{63}
$$

#### 2.3.1 Integration along the real axis: the limit of zero life-time broadening

Deforming the contour $\Gamma_1$ to the real axis such that the contributions from the Matsubara poles vanish and using relations in Eq. (60-61), Eq. (63) trivially reduces to

$$
\begin{aligned}
& \Sigma_{\mu\nu}(\vec{q},\varpi) = \\
& = \int_{-\infty}^{\infty} d\epsilon\; f(\epsilon)\; [\widetilde{\Sigma}_{\mu\nu}(\vec{q}; \epsilon+\hbar\omega+i\delta, \epsilon+i0) - \widetilde{\Sigma}_{\mu\nu}(-\vec{q}; \epsilon+\hbar\omega+i\delta, \epsilon-i0)] \\
& - \int_{-\infty}^{\infty} d\epsilon\; f(\epsilon)\; [\widetilde{\Sigma}_{\mu\nu}(\vec{q}; \epsilon-i0, \epsilon-\hbar\omega-i\delta) - \widetilde{\Sigma}_{\mu\nu}(-\vec{q}; \epsilon+i0, \epsilon-\hbar\omega-i\delta)] ,
\end{aligned}
\tag{64}
$$

or by inserting the definition of $\widetilde{\Sigma}_{\mu\nu}(\vec{q}; z_1, z_2)$,

$$
\begin{aligned}
& \Sigma_{\mu\nu}(\vec{q},\varpi) = \\
& -\frac{1}{2\pi V} \int_{-\infty}^{\infty} d\epsilon\; f(\epsilon)\; \Big( Tr\left\{ J_\mu(\vec{q})\; G(\epsilon+\hbar\omega+i\delta)\, J_\nu(-\vec{q})\; G^+(\epsilon) \right\} \\
& \qquad - Tr\left\{ J_\mu(-\vec{q})\; G(\epsilon+\hbar\omega+i\delta)\, J_\nu(\vec{q})\; G^-(\epsilon) \right\} \\
& \qquad - Tr\left\{ J_\mu(\vec{q})\; G^-(\epsilon)\, J_\nu(-\vec{q})\; G(\epsilon-\hbar\omega+i\delta) \right\} \\
& \qquad + Tr\left\{ J_\mu(-\vec{q})\; G^+(\epsilon)\, J_\nu(\vec{q})\; G(\epsilon-\hbar\omega-i\delta) \right\} \Big) ,
\end{aligned}
\tag{65}
$$

with the up- and down-side limits of the resolvent, $G^+(\epsilon)$ and $G^-(\epsilon)$, respectively. By taking the limit $\delta \rightarrow 0$, Eq. (65) transforms to

$$\begin{aligned}
&\Sigma_{\mu\nu}(\vec{q},\omega) = \qquad (66)\\
&-\frac{1}{2\pi V}\int_{-\infty}^{\infty} d\epsilon\; f(\epsilon)\; \Big( Tr\left\{J_\mu\left(\vec{q}\right)\, G^+(\epsilon+\hbar\omega)\, J_\nu\left(-\vec{q}\right)\, G^+(\epsilon)\right\} \\
&\qquad - Tr\left\{J_\mu\left(-\vec{q}\right)\, G^+(\epsilon+\hbar\omega)\, J_\nu\left(\vec{q}\right)\, G^-(\epsilon)\right\} \\
&\qquad - Tr\left\{J_\mu\left(\vec{q}\right)\, G^-(\epsilon)\, J_\nu\left(-\vec{q}\right)\, G^+(\epsilon+\hbar\omega)\right\} \\
&\qquad + Tr\left\{J_\mu\left(-\vec{q}\right)\, G^+(\epsilon)\, J_\nu\left(\vec{q}\right)\, G^-(\epsilon-\hbar\omega)\right\}\Big)\ .
\end{aligned}$$

In particular, for $\vec{q}=0$, Eq. (66) reduces to

$$\begin{aligned}
&\Sigma_{\mu\nu}(\omega) = \qquad (67)\\
&-\frac{1}{2\pi V}\int_{-\infty}^{\infty} d\epsilon\; f(\epsilon)\,\Big(\, Tr\left\{J_\mu\, G^+(\epsilon+\hbar\omega)\, J_\nu\, \left[G^+(\epsilon)-G^-(\epsilon)\right]\right\} \\
&\qquad + Tr\left\{J_\mu\, \left[G^+(\epsilon)-G^-(\epsilon)\right]\, J_\nu\, G^-(\epsilon-\hbar\omega)\right\}\Big)\ .
\end{aligned}$$

By shifting in the second term of Eq. (67) the argument of integration by $\hbar\omega$, the *Hermitean* part of $\Sigma_{\mu\nu}(\omega)$,

$$\mathrm{Re}\,\Sigma_{\mu\nu}(\omega) \equiv \frac{1}{2}(\Sigma_{\mu\nu}(\omega)+\Sigma_{\nu\mu}(\omega)^*)\ , \qquad (68)$$

can be expressed as

$$\begin{aligned}
&\mathrm{Re}\,\Sigma_{\mu\nu}(\omega) = \qquad (69)\\
&\frac{1}{\pi V}\int_{-\infty}^{\infty} d\epsilon\; (f(\epsilon)-f(\epsilon+\hbar\omega))\, Tr\left\{\, J_\mu\, \mathrm{Im}\, G^+(\epsilon+\hbar\omega)\, J_\nu\, \mathrm{Im}\, G^+(\epsilon)\right\}\ ,
\end{aligned}$$

with

$$\mathrm{Im}\, G^+(\epsilon) = \frac{1}{2i}\left(G^+(\epsilon)-G^-(\epsilon)\right)\ .$$

Since, quite clearly, $\mathrm{Re}\,\Sigma_{\mu\nu}(0)=0$,

$$\mathrm{Re}\,\sigma_{\mu\nu}(\omega) = \frac{\mathrm{Re}\,\Sigma_{\mu\nu}(\omega)}{\omega}\ , \qquad (70)$$

as used in practical calculations.

### 2.3.2 The static limit

In order to obtain the correct zero-frequency conductivity tensor, Eq. (65) has to be used in formula (43). Making use of the analyticity of the Green functions in the upper and lower complex semi-planes this leads to

$$\sigma_{\mu\nu} = -\frac{\hbar}{2\pi V}\int_{-\infty}^{\infty} d\epsilon\, f(\epsilon) \tag{71}$$
$$\times\, Tr\left\{ J^{\mu}\frac{\partial G^{+}(\epsilon)}{\partial\epsilon}J^{\nu}[G^{+}(\epsilon)-G^{-}(\epsilon)] - J^{\mu}[G^{+}(\epsilon)-G^{-}(\epsilon)]J^{\nu}\frac{\partial G^{-}(\epsilon)}{\partial\epsilon}\right\} \ .$$

Integrating by parts yields

$$\sigma_{\mu\nu} = -\int_{-\infty}^{\infty} d\epsilon\, \frac{df(\varepsilon)}{d\varepsilon} S_{\mu\nu}\left(\varepsilon\right) \ , \tag{72}$$

with

$$S_{\mu\nu}\left(\varepsilon\right) = -\frac{\hbar}{2\pi V}\int_{-\infty}^{\varepsilon} d\epsilon'$$
$$\times\, Tr\left\{ J^{\mu}\frac{\partial G^{+}(\epsilon')}{\partial\epsilon'}J^{\nu}[G^{+}(\epsilon')-G^{-}(\epsilon')] - J^{\mu}[G^{+}(\epsilon')-G^{-}(\epsilon')]J^{\nu}\frac{\partial G^{-}(\epsilon')}{\partial\epsilon'}\right\} \ , \tag{73}$$

which has the meaning of a zero-temperature, energy dependent conductivity. For $T = 0$, $\sigma_{\mu\nu}$ is obviously given by

$$\sigma_{\mu\nu} = S_{\mu\nu}\left(\varepsilon_F\right) \ . \tag{74}$$

A numerically tractable formula can be obtained for the *diagonal elements of the conductivity tensor*. Namely,

$$Tr\left\{ J^{\mu}\frac{\partial G^{+}(\epsilon)}{\partial\epsilon}J^{\mu}[G^{+}(\epsilon)-G^{-}(\epsilon)] - J^{\mu}[G^{+}(\epsilon)-G^{-}(\epsilon)]J^{\mu}\frac{\partial G^{-}(\epsilon)}{\partial\epsilon}\right\} =$$
$$= Tr\left\{ J^{\mu}\frac{\partial}{\partial\epsilon}\left[G^{+}(\epsilon)-G^{-}(\epsilon)\right] J^{\mu}[G^{+}(\epsilon)-G^{-}(\epsilon)]\right\}$$
$$= \frac{1}{2}\frac{\partial}{\partial\varepsilon}Tr\left\{ J^{\mu}[G^{+}(\epsilon)-G^{-}(\epsilon)]J^{\mu}[G^{+}(\epsilon)-G^{-}(\epsilon)]\right\} \ ,$$

thus, the widely used formula for the dc-conductivity

$$\sigma_{\mu\mu} = -\frac{\hbar}{4\pi V}Tr\left\{ J^{\mu}[G^{+}(\epsilon_F)-G^{-}(\epsilon_F)]J^{\mu}[G^{+}(\epsilon_F)-G^{-}(\epsilon_F)]\right\} \ , \tag{75}$$

is derived. It should be mentioned that by recalling the spectral resolution of the resolvents,

$$G^{+}(\epsilon)-G^{-}(\epsilon) = 2i\,\mathrm{Im}\,G^{+}(\epsilon) = -2i\pi\sum_{n}|n\rangle\langle n|\,\delta\left(\varepsilon-\varepsilon_n\right) \ , \tag{76}$$

Eq. (75) turns to be identical with the original Greenwood formula,

$$\sigma_{\mu\mu} = \frac{\pi\hbar}{V}\sum_{n,m} J^{\mu}_{nm}\, J^{\mu}_{mn}\,\delta\left(\varepsilon_F-\varepsilon_n\right)\,\delta\left(\varepsilon_F-\varepsilon_m\right) \ . \tag{77}$$

Alternatively, the static conductivity tensor, Eq. (71), can be recast according to Crépieux and Bruno, PRB **64** 014416 (2001) Appendix A. We start with the following identical manipulations,

$$
\begin{aligned}
&Tr\left\{J^{\mu}\frac{\partial G^{+}(\epsilon)}{\partial\epsilon}J^{\nu}[G^{+}(\epsilon)-G^{-}(\epsilon)]-J^{\mu}[G^{+}(\epsilon)-G^{-}(\epsilon)]J^{\nu}\frac{\partial G^{-}(\epsilon)}{\partial\epsilon}\right\}\\
&=Tr\left\{J^{\mu}\frac{\partial G^{+}(\epsilon)}{\partial\epsilon}J^{\nu}G^{+}(\epsilon)]+J^{\mu}G^{-}(\epsilon)J^{\nu}\frac{\partial G^{-}(\epsilon)}{\partial\epsilon}\right\}\\
&-Tr\left\{J^{\mu}\frac{\partial G^{+}(\epsilon)}{\partial\epsilon}J^{\nu}G^{-}(\epsilon)+J^{\mu}G^{+}(\epsilon)J^{\nu}\frac{\partial G^{-}(\epsilon)}{\partial\epsilon}\right\}
\end{aligned}
\tag{78}
$$

$$
\begin{aligned}
&=\frac{\partial}{\partial\epsilon}Tr\left\{J^{\mu}G^{+}(\epsilon)J^{\nu}G^{+}(\epsilon)+J^{\mu}G^{-}(\epsilon)J^{\nu}G^{-}(\epsilon)-J^{\mu}G^{+}(\epsilon)J^{\nu}G^{-}(\epsilon)\right\}\\
&-Tr\left\{J^{\mu}G^{+}(\epsilon)J^{\nu}\frac{\partial G^{+}(\epsilon)}{\partial\epsilon}+J^{\mu}\frac{\partial G^{-}(\epsilon)}{\partial\epsilon}J^{\nu}G^{-}(\epsilon)\right\}
\end{aligned}
\tag{79}
$$

$$
\begin{aligned}
&=-\frac{1}{2}\frac{\partial}{\partial\epsilon}Tr\left\{J^{\mu}\left[G^{+}(\epsilon)-G^{-}(\epsilon)\right]J^{\nu}G^{-}(\epsilon)-J^{\mu}G^{+}(\epsilon)J^{\nu}\left[G^{+}(\epsilon)-G^{-}(\epsilon)\right]\right\}\\
&+\frac{1}{2}\frac{\partial}{\partial\epsilon}Tr\left\{J^{\mu}G^{+}(\epsilon)J^{\nu}G^{+}(\epsilon)+J^{\mu}G^{-}(\epsilon)J^{\nu}G^{-}(\epsilon)\right\}\\
&-Tr\left\{J^{\mu}G^{+}(\epsilon)J^{\nu}\frac{\partial G^{+}(\epsilon)}{\partial\epsilon}+J^{\mu}\frac{\partial G^{-}(\epsilon)}{\partial\epsilon}J^{\nu}G^{-}(\epsilon)\right\}
\end{aligned}
\tag{80}
$$

$$
\begin{aligned}
&=-\frac{1}{2}\frac{\partial}{\partial\epsilon}Tr\left\{J^{\mu}\left[G^{+}(\epsilon)-G^{-}(\epsilon)\right]J^{\nu}G^{-}(\epsilon)-J^{\mu}G^{+}(\epsilon)J^{\nu}\left[G^{+}(\epsilon)-G^{-}(\epsilon)\right]\right\}\\
&+\frac{1}{2}Tr\left\{J^{\mu}\frac{\partial G^{+}(\epsilon)}{\partial\epsilon})J^{\nu}G^{+}(\epsilon)-J^{\mu}G^{+}(\epsilon)J^{\nu}\frac{\partial G^{+}(\epsilon)}{\partial\epsilon}\right.\\
&\qquad\left.J^{\mu}G^{-}(\epsilon)J^{\nu}\frac{\partial G^{-}(\epsilon)}{\partial\epsilon}-J^{\mu}\frac{\partial G^{-}(\epsilon)}{\partial\epsilon}J^{\nu}G^{-}(\epsilon)\right\}\ .
\end{aligned}
\tag{81}
$$

Utilyzing $\frac{\partial G^{\pm}(\epsilon)}{\partial\epsilon}=-G^{\pm}(\epsilon)^{2}$, the second term can be rewritten as

$$
\begin{aligned}
&-\frac{1}{2}Tr\left\{J^{\mu}G^{+}(\epsilon)^{2}J^{\nu}G^{+}(\epsilon)-J^{\mu}G^{+}(\epsilon)J^{\nu}G^{+}(\epsilon)^{2}\right.\\
&\qquad\left.+J^{\mu}G^{-}(\epsilon)J^{\nu}G^{-}(\epsilon)^{2}-J^{\mu}G^{-}(\epsilon)^{2}J^{\nu}G^{-}(\epsilon)\right\}\ .
\end{aligned}
\tag{82}
$$

Since

$$
J^{\mu}=-ec\alpha^{\mu}=\frac{ei}{\hbar}\left[x^{\mu},H\right]=-\frac{ei}{\hbar}\left[x^{\mu},G^{\pm}\left(\varepsilon\right)^{-1}\right]=\frac{ei}{\hbar}\left(G^{\pm}\left(\varepsilon\right)^{-1}x^{\mu}-x^{\mu}G^{\pm}\left(\varepsilon\right)^{-1}\right)\ ,\tag{83}
$$

thus,

$$
Tr\left\{J^{\mu}G^{\pm}(\epsilon)^{2}J^{\nu}G^{\pm}(\epsilon)\right\}=\frac{ei}{\hbar}Tr\left\{J^{\mu}G^{\pm}(\epsilon)x^{\nu}G^{\pm}(\epsilon)-J^{\mu}G^{\pm}(\epsilon)^{2}x^{\nu}\right\}\tag{84}
$$

$$
Tr\left\{J^{\mu}G^{\pm}(\epsilon)J^{\nu}G^{\pm}(\epsilon)^{2}\right\}=Tr\left\{G^{\pm}(\epsilon)J^{\mu}G^{\pm}(\epsilon)J^{\nu}G^{\pm}(\epsilon)\right\}\tag{85}
$$

$$
=\frac{ei}{\hbar}Tr\left\{x^{\mu}G^{\pm}(\epsilon)J^{\nu}G^{\pm}(\epsilon)-G^{\pm}(\epsilon)^{2}x^{\mu}J^{\nu}\right\}\ ,\tag{86}
$$

this term can further be rewritten as,

$$\frac{ei}{2\hbar}Tr\left\{x^\mu G^+(\epsilon)J^\nu G^+(\epsilon) - G^+(\epsilon)^2 x^\mu J^\nu - J^\mu G^+(\epsilon)x^\nu G^+(\epsilon) + G^+(\epsilon)^2 x^\nu J^\mu\right. \tag{87}$$

$$\left. -x^\mu G^-(\epsilon)J^\nu G^-(\epsilon) + G^-(\epsilon)^2 x^\mu J^\nu + J^\mu G^-(\epsilon)x^\nu G^-(\epsilon) - G^\pm(\epsilon)^2 x^\nu J^\mu\right\}$$

$$= -\frac{ei}{2\hbar}\frac{\partial}{\partial\varepsilon}Tr\left\{\left(G^+(\epsilon) - G^-(\epsilon)\right)(x^\mu J^\nu - x^\nu J^\mu)\right\} \tag{88}$$

$$-\frac{ei}{2\hbar}\,\mathrm{Re}\,Tr\left\{x^\mu G^+(\epsilon)J^\nu G^+(\epsilon) - J^\mu G^+(\epsilon)x^\nu G^+(\epsilon)\right\}\ .$$

Here we used,

$$Tr\left\{x^\mu G^+(\epsilon)J^\nu G^+(\epsilon)\right\}^* = Tr\left\{x^\mu G^-(\epsilon)J^\nu G^-(\epsilon)\right\}\ . \tag{89}$$

Collecting all terms, the static conductivity tensor can be written as

$$\sigma_{\mu\nu} = \frac{\hbar}{4\pi V}Tr\left\{J^\mu\left[G^+(\epsilon_F) - G^-(\epsilon_F)\right]J^\nu G^-(\epsilon_F) - J^\mu G^+(\epsilon_F)J^\nu\left[G^+(\epsilon_F) - G^-(\epsilon_F)\right]\right\}$$
$$-\frac{e}{4i\pi V}Tr\left\{\left(G^+(\epsilon_F) - G^-(\epsilon_F)\right)(x^\mu J^\nu - x^\nu J^\mu)\right\}$$
$$-\frac{e}{4i\pi V}\,\mathrm{Re}\int_{-\infty}^{\varepsilon_F} d\epsilon' Tr\left\{x^\mu G^+(\epsilon')J^\nu G^+(\epsilon') - J^\mu G^+(\epsilon')x^\nu G^+(\epsilon')\right\}\ . \tag{90}$$

The first to terms are clearly identical with $\sigma^I_{\mu\nu}$ and $\sigma^{II}_{\mu\nu}$ as given in Eqs. (A14) and (A15) of Crépieux and Bruno, respectively, while the third term can be shown to be zero (*I. Turek, private communication*). Namely, by using Eq. (83),

$$Tr\left\{x^\mu G(z)J^\nu G(z) - J^\mu G(z)x^\nu G(z)\right\}$$
$$= \frac{ei}{\hbar}Tr\left\{x^\mu G(z)\left(G(z)^{-1}x^\nu - x^\nu G(z)^{-1}\right)G(z) - \left(G(z)^{-1}x^\mu - x^\mu G(z)^{-1}\right)G(z)x^\nu G(z)\right\}$$
$$= \frac{ei}{\hbar}\left[Tr\left\{x^\mu x^\nu G(z)\right\} - Tr\left\{x^\mu G(z)x^\nu\right\} - Tr\left\{x^\mu x^\nu G(z)\right\} + Tr\left\{x^\mu G(z)x^\nu\right\}\right] = 0\ . \tag{91}$$

The final expression of the static conductivity tensor, therefore, reads as

$$\sigma_{\mu\nu} = \frac{\hbar}{4\pi V}Tr\left\{J^\mu\left[G^+(\epsilon_F) - G^-(\epsilon_F)\right]J^\nu G^-(\epsilon_F) - J^\mu G^+(\epsilon_F)J^\nu\left[G^+(\epsilon_F) - G^-(\epsilon_F)\right]\right\}$$
$$+\frac{ie}{4\pi V}Tr\left\{\left(G^+(\epsilon_F) - G^-(\epsilon_F)\right)(x^\mu J^\nu - x^\nu J^\mu)\right\}\ . \tag{92}$$

# 3 CPA condition for layered systems

Consider a layered system, which at best has only two-dimensional translational symmetry. Suppose such a layered system corresponds to a parent infinite (three-dimensional periodic) system consisting of a simple lattice with only one atom per unit cell, then any lattice site $\vec{R}_{pi}$ can be written as

$$\vec{R}_{pi} = \vec{C}_p + \vec{R}_i \quad ; \quad \vec{R}_i \in L_2 \quad , \tag{93}$$

where $\vec{C}_p$ is the "spanning vector" of a particular layer $p$ and the two-dimensional (real) lattice is denoted by $L_2 = \left\{ \vec{R}_i \right\}$ with the corresponding set of indices $I(L_2)$. For a given interface region of $n$ layers, containing also disordered layers, the coherent scattering path operator $\boldsymbol{\tau}_c(z)$ is given by the following Surface Brillouin Zone ($SBZ$-) integral,

$$\underline{\tau}_c^{pi,qj}(z) = \Omega_{SBZ}^{-1} \int \exp\left(-i\vec{k}\cdot(\vec{R}_i - \vec{R}_j)\right) \widehat{\underline{\tau}}_c^{pq}(\vec{k}, z)\, d^2k \quad , \tag{94}$$

which implies two–dimensional translational invariance of the coherent medium for all layers of the interface region, i.e., that in each layer $p$ for the coherent single–site $t$–matrices the following translational invariance applies:

$$\underline{t}_c^{pi}(z) = \widehat{\underline{t}}_c^{p}(z) \quad ; \quad \forall i \in I(L_2) \quad . \tag{95}$$

It should be noted that all scattering path operators are angular momentum representations reflecting either a non-relativistic or a relativistic description of multiple scattering. Numerical recipes to evaluate $\widehat{\underline{\tau}}_c^{pq}(\vec{k}, z)$ in (94) for layered structures are provided by different variants of multiple scattering theory. In the following supermatrices labelled by layers only and denoted by a 'hat' symbol will be used:

$$\widehat{\mathbf{t}}_c(z) = \begin{pmatrix} \widehat{\underline{t}}_c^{1}(z) & 0 & \cdots & & 0 \\ & \ddots & & & \\ 0 & \cdots & \widehat{\underline{t}}_c^{p}(z) & \cdots & 0 \\ & & & \ddots & \\ 0 & & \cdots & 0 & \widehat{\underline{t}}_c^{n}(z) \end{pmatrix} \quad , \tag{96}$$

and

$$\widehat{\boldsymbol{\tau}}_c(z) = \begin{pmatrix} & \vdots & & \vdots & \\ \cdots & \widehat{\underline{\tau}}_c^{pp}(z) & \cdots & \widehat{\underline{\tau}}_c^{pq}(z) & \cdots \\ & \vdots & & \vdots & \\ \cdots & \widehat{\underline{\tau}}_c^{qp}(z) & \cdots & \widehat{\underline{\tau}}_c^{qq}(z) & \cdots \\ & \vdots & & \vdots & \end{pmatrix} \quad , \tag{97}$$

$$p, q = 1, \ldots, n \quad .$$

Quite clearly, a particular element of $\widehat{\boldsymbol{\tau}}_c(z)$,

$$\widehat{\underline{\tau}}_c^{pq}(z) = \underline{\tau}_c^{pi,qi}(z) = \underline{\tau}_c^{p0,q0}(z) = \Omega_{SBZ}^{-1} \int \widehat{\tau}_c^{pq}(\vec{k}, z)\, d^2k \quad , \tag{98}$$

refers to the unit cells at the origin of $L_2$ in layers $p$ and $q$. Suppose now the concentration for constituents $A$ and $B$ in layer $p$ is denoted by $c_p^\alpha$ $(p=1,\ldots,n)$. The corresponding layer-diagonal element of the so-called impurity matrix, that specifies a single impurity of type $\alpha$ in the translational invariant "host" formed by layer $p$, is then given by

$$\widehat{\underline{D}}_\alpha^p(z) \equiv \underline{D}_\alpha^{p0}(z) = \left[\underline{I} - \underline{m}_\alpha^{p0}(z)\underline{\tau}_c^{p0,p0}(z)\right]^{-1} \quad , \tag{99}$$

with

$$\underline{m}_\alpha^{pi}(z) = \underline{m}_\alpha^{p0}(z) = \widehat{\underline{m}}_\alpha^p(z) = \widehat{\underline{t}}_c^p(z)^{-1} - \widehat{\underline{t}}_\alpha^p(z)^{-1}, \quad \alpha = A, B \quad , \tag{100}$$

where $\widehat{\underline{t}}_\alpha^p(z)$ is the single–site $t$–matrix for constituent $\alpha$ in layer $p$. The coherent scattering path operator for the interface region $\widehat{\boldsymbol{\tau}}_c(z)$, is therefore obtained from the following inhomogeneous CPA condition,

$$\widehat{\underline{\tau}}_c^{pp}(z) = \sum_{\alpha=A,B} c_p^\alpha \left\langle \widehat{\underline{\tau}}^{pp}(z) \right\rangle_{p,\alpha} \quad , \tag{101}$$

$$\left\langle \widehat{\underline{\tau}}^{pp}(z) \right\rangle_{p,\alpha} = \widehat{\underline{\tau}}_\alpha^{pp}(z) = \widehat{\underline{D}}_\alpha^p(z)\widehat{\underline{\tau}}_c^{pp}(z) \quad , \tag{102}$$

i.e., from a condition that implies solving *simultaneously* a layer-diagonal CPA condition for layers $p=1,\ldots,n$. Once this condition is met then translational invariance in each layer under consideration is achieved,

$$\left\langle \widehat{\underline{\tau}}^{pp}(z) \right\rangle_{p,\alpha} \equiv \left\langle \underline{\tau}^{p0,p0}(z) \right\rangle_{p0,\alpha} = \left\langle \underline{\tau}^{pi,pi}(z) \right\rangle_{pi,\alpha} \quad , \tag{103}$$
$$\forall i \in I(L_2) \quad , \quad p=1,\ldots,n \quad .$$

Similarly, by specifying the occupation on two different sites the following restricted averages are obtained,

$$p \neq q: \quad \left\langle \underline{\tau}^{pi,qj}(z) \right\rangle_{pi\alpha,qj\beta} = \widehat{\underline{D}}_\alpha^p(z)\underline{\tau}_c^{pi,qj}(z)\widehat{\underline{D}}_\beta^q(z)^t \quad , \tag{104}$$

$$p = q,\ i \neq j: \quad = \left\langle \underline{\tau}^{pi,pj}(z) \right\rangle_{pi\alpha,pj\beta} = \widehat{\underline{D}}_\alpha^p(z)\underline{\tau}_c^{pi,pj}(z)\widehat{\underline{D}}_\beta^p(z)^t \quad , \tag{105}$$

where $\langle \underline{\tau}_c^{pi,qj}(z) \rangle_{pi\alpha,qj\beta}$ has the meaning that site (subcell) $pi$ is occupied by species $\alpha$ and site (subcell) $qj$ by species $\beta$ and the symbol $t$ indicates a transposed matrix.

# 4 Conductivity for disordered layered systems

## 4.1 General expressions

Suppose the electrical conductivity of a disordered system, namely $\sigma_{\mu\mu}$, is calculated using the Kubo-Greenwood formula (77)

$$\sigma_{\mu\mu} = \frac{\pi\hbar}{N_0 V_{at}} \left\langle \sum_{m,n} J^{\mu}_{mn} J^{\mu}_{nm} \delta(\varepsilon_F - \varepsilon_m)\delta(\varepsilon_F - \varepsilon_n) \right\rangle \quad , \tag{106}$$

where $N_0$ is the number of atoms, $V_{at}$ is the atomic volume, and $\langle \cdots \rangle$ denotes an average over configurations. As we have seen, Eq. (106) can be reformulated in terms of the imaginary part of the (one-particle) Green function

$$\sigma_{\mu\mu} = \frac{\hbar}{\pi N_0 V_{at}} Tr \ \left\langle J_\mu \operatorname{Im} G^+(\varepsilon_F) J_\mu \operatorname{Im} G^+(\varepsilon_F) \right\rangle \quad . \tag{107}$$

By using "up-" and "down-" side limits, Eq. (107) can be rewritten as

$$\sigma_{\mu\mu} = \frac{1}{4} \left\{ \widetilde{\sigma}_{\mu\mu}(\varepsilon^+, \varepsilon^+) + \widetilde{\sigma}_{\mu\mu}(\varepsilon^-, \varepsilon^-) - \ \widetilde{\sigma}_{\mu\mu}(\varepsilon^+, \varepsilon^-) - \widetilde{\sigma}_{\mu\mu}(\varepsilon^-, \varepsilon^+) \right\} \quad , \tag{108}$$

where

$$\varepsilon^+ = \varepsilon_F + i\delta \quad , \quad \varepsilon^- = \varepsilon_F - i\delta \quad ; \quad \delta \to +0 \quad ,$$

and

$$\widetilde{\sigma}_{\mu\mu}(\varepsilon_1, \varepsilon_2) = -\frac{\hbar}{\pi N_0 V_{at}} Tr \ \langle J_\mu G(\varepsilon_1) J_\mu G(\varepsilon_2) \rangle \quad . \tag{109}$$

$$\big(\varepsilon_i \in \left\{\varepsilon^+, \varepsilon^-\right\} \quad ; \quad i = 1, 2\big)$$

Employing the expression of the Green function within the KKR method, a typical contribution to the conductivity can be expressed in terms of real space scattering path operators,

$$\widetilde{\sigma}_{\mu\mu}(\varepsilon_1, \varepsilon_2) = \tag{110}$$

$$= \frac{C}{N_0} \sum_{p=1}^{n} \left\{ \sum_{i \in I(L_2)} \sum_{q=1}^{n} \left\{ \sum_{j \in I(L_2)} tr \left\langle \underline{J}^{pi}_{\mu}(\varepsilon_2, \varepsilon_1) \underline{\tau}^{pi,qj}(\varepsilon_1) \underline{J}^{qj}_{\mu}(\varepsilon_1, \varepsilon_2) \underline{\tau}^{qj,pi}(\varepsilon_2) \right\rangle \right\} \right\} \quad ,$$

where $C = -\ (4m^2/\hbar^3 \pi V_{at})$, $N_0 = nN$ is the total number of sites in the interface region, as given in terms of the number of layers in the interface region ($n$) and the order of the two-dimensional translational group $N$ (number of atoms in one layer) and $tr$ denotes now the trace in angular momentum space. Let $\underline{J}^{p\alpha}_{\mu}(\varepsilon_1, \varepsilon_2)$ denote the angular momentum representation of the $\mu-$th component of the current operator according to component $\alpha = A, B$ in a particular layer $p$. Using a non-relativistic formulation for the current operator, namely $\vec{J} = (e\hbar/im)\,\vec{\nabla}$, the elements of $\underline{J}_{\mu}^{p\alpha}(\epsilon_1, \epsilon_2)$ are given by

$$
\begin{aligned}
& J^{p\alpha}_{\mu,\Lambda\Lambda'}(\varepsilon_1,\varepsilon_2) = \\
& = \frac{e}{m}\frac{\hbar}{i}\int\limits_{WS} Z^{p\alpha}_{\Lambda}(\varepsilon_1;\vec{r}_{p0})^{\times}\frac{\partial}{\partial r_{p0,\mu}} Z^{p\alpha}_{\Lambda'}(\varepsilon_2;\vec{r}_{p0})\, d^3 r_{p0} \ , \quad (\Lambda = (\ell, m)) \ ,
\end{aligned}
\tag{111}
$$

while within a relativistic formulation for the current operator, namely $\vec{J} = ec\vec{\alpha}$, one gets

$$
\begin{aligned}
& J^{p\alpha}_{\mu,\Lambda\Lambda'}(\varepsilon_1,\varepsilon_2) = \\
& = ec\int\limits_{WS} Z^{p\alpha}_{\Lambda}(\varepsilon_1;\vec{r}_{p0})^{\times}\alpha_{\mu}\, Z^{p\alpha}_{\Lambda'}(\varepsilon_2;\vec{r}_{p0})\, d^3 r_{p0} \ , \quad (\Lambda = (\ell, j, m_j)) \ .
\end{aligned}
\tag{112}
$$

In Eqs. (111) and (112) the functions $Z^{p\alpha}_{\Lambda}(\varepsilon_i;\vec{r}_{p0})$ are regular scattering solutions and $WS$ denotes the volume of the Wigner-Seitz sphere. It should also be noted that

$$
\underline{J}_{\mu}^{p\alpha}(\varepsilon_1,\varepsilon_2) = \underline{J}_{\mu}^{p0,\alpha}(\varepsilon_1,\varepsilon_2) = \underline{J}_{\mu}^{pi,\alpha}(\varepsilon_1,\varepsilon_2) \quad , \quad \forall i \in I(L_2) \quad . \tag{113}
$$

From the brackets in (110), one easily can see that for each layer $p$ the first sum over $L_2$ yields $N$ times the same contribution, provided two-dimensional invariance applies in all layers under consideration. Asumming this kind of symmetry, a typical contribution $\widetilde{\sigma}_{\mu\mu}(\varepsilon_1,\varepsilon_2)$ to the conductivity is therefore given by

$$
\begin{aligned}
& \widetilde{\sigma}_{\mu\mu}(\varepsilon_1,\varepsilon_2) = \\
& = \frac{C}{n}\sum_{p=1}^{n}\sum_{q=1}^{n}\left\{\sum_{j\in I(L_2)} tr\left\langle \underline{J}_{\mu}^{p0}(\varepsilon_2,\varepsilon_1)\underline{\tau}^{p0,qj}(\varepsilon_1)\underline{J}_{\mu}^{qj}(\varepsilon_1,\varepsilon_2)\underline{\tau}^{qj,p0}(\varepsilon_2)\right\rangle\right\} \quad ,
\end{aligned}
\tag{114}
$$

where $p0$ specifies the origin of $L_2$ for the $p$-th layer. This kind of contribution can be split up into a (site-) diagonal and a (site-) off-diagonal part,

$$
\widetilde{\sigma}_{\mu\mu}(\varepsilon_1,\varepsilon_2) = \widetilde{\sigma}^0_{\mu\mu}(\varepsilon_1,\varepsilon_2) + \widetilde{\sigma}^1_{\mu\mu}(\varepsilon_1,\varepsilon_2) \quad . \tag{115}
$$

## 4.2 Site-diagonal conductivity

By employing the CPA condition in (101) and *omitting vertex corrections*, for the diagonal part ($p0 = qj$) one simply gets in terms of the definitions given in (103) and (105),

$$
\begin{aligned}
&\widetilde{\sigma}^0_{\mu\mu}(\varepsilon_1,\varepsilon_2) = \\
&= \frac{C}{n}\sum_{p=1}^{n}\sum_{\alpha=A,B} c_p^\alpha tr\left[\underline{J}^{p\alpha}_\mu(\varepsilon_2,\varepsilon_1)\left\langle\widehat{\underline{\tau}}^{pp}(\varepsilon_1)\right\rangle_{p\alpha}\underline{J}^{p\alpha}_\mu(\varepsilon_1,\varepsilon_2)\left\langle\widehat{\underline{\tau}}^{pp}(\varepsilon_2)\right\rangle_{p\alpha}\right] \\
&= \frac{C}{n}\sum_{p=1}^{n}\sum_{\alpha=A,B} c_p^\alpha tr\left[\underline{J}^{p\alpha}_\mu(\varepsilon_2,\varepsilon_1)\widehat{\underline{D}}^p_\alpha(\varepsilon_1)\widehat{\underline{\tau}}^{pp}_c(\varepsilon_1)\underline{J}^{p\alpha}_\mu(\varepsilon_1,\varepsilon_2)\widehat{\underline{D}}^p_\alpha(\varepsilon_2)\widehat{\underline{\tau}}^{pp}_c(\varepsilon_2)\right] \\
&= \frac{C}{n}\sum_{p=1}^{n}\sum_{\alpha=A,B} c_p^\alpha tr\left[\widetilde{\underline{J}}^{p\alpha}_\mu(\varepsilon_2,\varepsilon_1)\widehat{\underline{\tau}}^{pp}_c(\varepsilon_1)\underline{J}^{p\alpha}_\mu(\varepsilon_1,\varepsilon_2)\widehat{\underline{\tau}}^{pp}_c(\varepsilon_2)\right]\ ,
\end{aligned}
\tag{116}
$$

where

$$
\widetilde{\underline{J}}^{p\alpha}_\mu(\varepsilon_2,\varepsilon_1) = \widehat{\underline{D}}^p_\alpha(\varepsilon_2)^t\underline{J}^{p\alpha}_\mu(\varepsilon_2,\varepsilon_1)\widehat{\underline{D}}^p_\alpha(\varepsilon_1)\ . \tag{117}
$$

## 4.3 Site-off-diagonal conductivity

According to (105) and (104) the off-diagonal part can further be partitioned into two terms,

$$
\widetilde{\sigma}^1_{\mu\mu}(\varepsilon_1,\varepsilon_2) = \widetilde{\sigma}^2_{\mu\mu}(\varepsilon_1,\varepsilon_2) + \widetilde{\sigma}^3_{\mu\mu}(\varepsilon_1,\varepsilon_2) \quad , \tag{118}
$$

where

$$
\begin{aligned}
&\widetilde{\sigma}^2_{\mu\mu}(\varepsilon_1,\varepsilon_2) = \\
&\frac{C}{n}\sum_{p=1}^{n}\sum_{q=1}^{n}(1-\delta_{pq})\left\{\sum_{j\in I(L_2)} tr\left\langle\underline{J}^{p0}_\mu(\varepsilon_2,\varepsilon_1)\underline{\tau}^{p0,qj}(\varepsilon_1)\underline{J}^{qj}_\mu(\varepsilon_1,\varepsilon_2)\underline{\tau}^{qj,p0}(\varepsilon_2)\right\rangle\right\}\ ,
\end{aligned}
\tag{119}
$$

and

$$
\begin{aligned}
&\widetilde{\sigma}^3_{\mu\mu}(\varepsilon_1,\varepsilon_2) = \\
&\frac{C}{n}\sum_{p=1}^{n}\sum_{q=1}^{n}\delta_{pq}\left\{\sum_{(j\neq 0)\in I(L_2)} tr\left\langle\underline{J}^{p0}_\mu(\varepsilon_2,\varepsilon_1)\underline{\tau}^{p0,qj}(\varepsilon_1)\underline{J}^{qj}_\mu(\varepsilon_1,\varepsilon_2)\underline{\tau}^{qj,p0}(\varepsilon_2)\right\rangle\right\}\ .
\end{aligned}
\tag{120}
$$

As one can see $\widetilde{\sigma}^2_{\mu\mu}(\varepsilon_1,\varepsilon_2)$ arises from pairs of sites located in *different* layers, whereas $\widetilde{\sigma}^3_{\mu\mu}(\varepsilon_1,\varepsilon_2)$ corresponds to pairs of sites in *one and the same* layer (excluding the site-diagonal pair already being accounted for in $\widetilde{\sigma}^0_{\mu\mu}(\varepsilon_1,\varepsilon_2)$). In general the averaging of $\widetilde{\sigma}^2_{\mu\mu}(\varepsilon_1,\varepsilon_2)$ is given by

$$
\begin{aligned}
\widetilde{\sigma}^2_{\mu\mu}(\varepsilon_1,\varepsilon_2) &= \frac{C}{n}\sum_{p=1}^{n}\sum_{q=1}^{n}(1-\delta_{pq})\sum_{j\in I(L_2)}\sum_{\alpha,\beta=A,B} c_p^\alpha c_q^\beta \\
&\times\ tr\left\{\underline{J}^{p\alpha}_\mu(\varepsilon_2,\varepsilon_1)\left\langle\underline{\tau}^{p0,qj}(\varepsilon_1)J^{qj}_\mu(\varepsilon_1,\varepsilon_2)\underline{\tau}^{qj,p0}(\varepsilon_2)\right\rangle_{p0\alpha,qj\beta}\right\}\ .
\end{aligned}
\tag{121}
$$

By employing the CPA condition and omitting vertex corrections, $\widetilde{\sigma}^2_{\mu\mu}(\varepsilon_1,\varepsilon_2)$ is found to reduce to

$$\widetilde{\sigma}^2_{\mu\mu}(\varepsilon_1,\varepsilon_2) = \frac{C}{n}\sum_{p=1}^{n}\sum_{q=1}^{n}(1-\delta_{pq})\sum_{j\in I(L_2)}\sum_{\alpha,\beta=A,B} c_p^\alpha c_q^\beta$$
$$\times\ tr\left\{\underline{J}_\mu^{p\alpha}(\varepsilon_2,\varepsilon_1)\left\langle\underline{\tau}^{p0,qj}(\varepsilon_1)\right\rangle_{p0a,qj\beta}\underline{J}_\mu^{q\beta}(\varepsilon_1,\varepsilon_2)\left\langle\underline{\tau}^{qj,p0}(\varepsilon_2)\right\rangle_{p0\alpha,qj\beta}\right\}\ , \tag{122}$$

or, by using (104), to

$$\widetilde{\sigma}^2_{\mu\mu}(\varepsilon_1,\varepsilon_2) = \frac{C}{n}\sum_{p=1}^{n}\sum_{q=1}^{n}(1-\delta_{pq})\sum_{j\in I(L_2)}\sum_{\alpha,\beta=A,B} c_p^\alpha c_q^\beta$$
$$\times\ tr\left\{\underline{\widetilde{J}}_\mu^{p\alpha}(\varepsilon_2,\varepsilon_1)\underline{\tau}_c^{p0,qj}(\varepsilon_1)\underline{\widetilde{J}}_\mu^{q\beta}(\varepsilon_1,\varepsilon_2)\underline{\tau}_c^{qj,p0}(\varepsilon_2)\right\}\ . \tag{123}$$

Since the site-off-diagonal scattering path operators $\tau_c^{p0,qj}(z)$ are defined as

$$\underline{\tau}_c^{p0,qj}(z) = \Omega_{SBZ}^{-1}\int e^{i\vec{k}\cdot\vec{R}_j}\underline{\widehat{\tau}}^{pq}(\vec{k},z)\,d^2k \quad , \tag{124}$$

the orthogonality for irreducible representations of the two-dimensional translation group can be used:

$$\sum_{j\in I(L_2)}\underline{\tau}_c^{p0,qj}(\varepsilon_1)\underline{\tau}_c^{qj,p0}(\varepsilon_2) = \Omega_{SBZ}^{-1}\int\underline{\widehat{\tau}}^{pq}(\vec{k},\varepsilon_1)\widehat{\tau}^{qp}(\vec{k},\varepsilon_2)d^2k \quad . \tag{125}$$

For $\widetilde{\sigma}^2_{\mu\mu}(\varepsilon_1,\varepsilon_2)$ one therefore gets the following expression,

$$\widetilde{\sigma}^2_{\mu\mu}(\varepsilon_1,\varepsilon_2) = \frac{C}{n\Omega_{SBZ}}\sum_{p=1}^{n}\sum_{q=1}^{n}(1-\delta_{pq})\sum_{\alpha,\beta=A,B} c_p^\alpha c_q^\beta \tag{126}$$
$$\times\int tr\left\{\underline{\widetilde{J}}_\mu^{p\alpha}(\varepsilon_2,\varepsilon_1)\underline{\widehat{\tau}}_c^{pq}(\vec{k},\varepsilon_1)\underline{\widetilde{J}}_\mu^{q\beta}(\varepsilon_1,\varepsilon_2)\underline{\widehat{\tau}}_c^{qp}(\vec{k},\varepsilon_2)\right\}\,d^2k\ .$$

From the above discussion of $\widetilde{\sigma}^2_{\mu\mu}(\varepsilon_1,\varepsilon_2)$ it is easy to see that $\widetilde{\sigma}^3_{\mu\mu}(\varepsilon_1,\varepsilon_2)$ is given by

$$\widetilde{\sigma}^3_{\mu\mu}(\varepsilon_1,\varepsilon_2) = \frac{C}{n\Omega_{SBZ}}\sum_{p=1}^{n}\sum_{\alpha,\beta=A,B} c_p^\alpha c_p^\beta \tag{127}$$
$$\times\int tr\left\{\underline{\widetilde{J}}_\mu^{p\alpha}(\varepsilon_2,\varepsilon_1)\underline{\widehat{\tau}}_c^{pp}(\vec{k},\varepsilon_1)\underline{\widetilde{J}}_\mu^{p\beta}(\varepsilon_1,\varepsilon_2)\underline{\widehat{\tau}}_c^{pp}(\vec{k},\varepsilon_2)\right\}\,d^2k$$
$$+\ \widetilde{\sigma}^{3,corr}_{\mu\mu}(\varepsilon_1,\varepsilon_2)\ ,$$

where $\widetilde{\sigma}^{3,corr}_{\mu\mu}(\varepsilon_1,\varepsilon_2)$ arises from extending the sum in (120) to $\forall j\in I(L_2)$ and subtracting a corresponding correction term of the form,

$$\widetilde{\sigma}^{3,corr}_{\mu\mu}(\varepsilon_1,\varepsilon_2) =$$
$$= -\frac{C}{n}\sum_{p=1}^{n}\sum_{\alpha,\beta=A,B} c_p^\alpha c_p^\beta\, tr\left\{\underline{J}^{p\alpha}_\mu(\varepsilon_2,\varepsilon_1)\underline{\widehat{D}}^p_\alpha(\varepsilon_1)\underline{\widehat{\tau}}^{pp}_c(\varepsilon_1)\underline{\widehat{D}}^p_\beta(\varepsilon_1)^t \right.$$
$$\left. \times\ \underline{J}^{p\beta}_\mu(\varepsilon_1,\varepsilon_2)\underline{\widehat{D}}^p_\beta(\varepsilon_2)\underline{\widehat{\tau}}^{pp}_c(\varepsilon_2)\underline{\widehat{D}}^p_\alpha(\varepsilon_2)^t\right\}$$
$$= -\frac{C}{n}\sum_{p=1}^{n}\sum_{\alpha,\beta=A,B} c_p^\alpha c_p^\beta\, tr\left\{\underline{\widetilde{J}}^{p\alpha}_\mu(\varepsilon_2,\varepsilon_1)\underline{\widehat{\tau}}^{pp}_c(\varepsilon_1)\underline{\widetilde{J}}^{p\beta}_\mu(\varepsilon_1,\varepsilon_2)\underline{\widehat{\tau}}^{pp}_c(\varepsilon_2)\right\}\ . \tag{128}$$

## 4.4 Total conductivity for layered systems

Combining now all terms, a typical contribution $\widetilde{\sigma}_{\mu\mu}(\varepsilon_1,\varepsilon_2)$ to the conductivity is given by

$$\widetilde{\sigma}_{\mu\mu}(\varepsilon_1,\varepsilon_2) = \tag{129}$$
$$= \frac{C}{n}\sum_{p=1}^{n}\left(\sum_{\alpha=A,B} c_p^\alpha\, tr\left\{\underline{\widetilde{J}}^{p\alpha}_\mu(\varepsilon_2,\varepsilon_1)\underline{\widehat{\tau}}^{pp}_c(\varepsilon_1)\underline{J}^{p\alpha}_\mu(\varepsilon_1,\varepsilon_2)\underline{\widehat{\tau}}^{pp}_c(\varepsilon_2)\right\}\right.$$
$$- \sum_{\alpha,\beta=A,B} c_p^\alpha c_p^\beta\, tr\left\{\underline{\widetilde{J}}^{p\alpha}_\mu(\varepsilon_2,\varepsilon_1)\underline{\widehat{\tau}}^{pp}_c(\varepsilon_1)\underline{\widetilde{J}}^{p\beta}_\mu(\varepsilon_1,\varepsilon_2)\underline{\widehat{\tau}}^{pp}_c(\varepsilon_2)\right\}$$
$$\left. + \Omega_{SBZ}^{-1}\sum_{q=1}^{n}\sum_{\alpha,\beta=A,B} c_p^\alpha c_q^\beta \int tr\left\{\underline{\widetilde{J}}^{p\alpha}_\mu(\varepsilon_2,\varepsilon_1)\underline{\widehat{\tau}}^{pq}_c(\vec{k},\varepsilon_1)\underline{\widetilde{J}}^{q\beta}_\mu(\varepsilon_1,\varepsilon_2)\underline{\widehat{\tau}}^{qp}_c(\vec{k},\varepsilon_2)\right\} d^2k\right)\ ,$$

which, as far as the summations over layers are consered, can be partitioned into 'single' and 'double' terms,

$$\widetilde{\sigma}_{\mu\mu}(\varepsilon_1,\varepsilon_2) = \sum_{p=1}^{n}\widetilde{\sigma}^{p}_{\mu\mu}(\varepsilon_1,\varepsilon_2) + \sum_{p,q=1}^{n}\widetilde{\sigma}^{pq}_{\mu\mu}(\varepsilon_1,\varepsilon_2)\ . \tag{130}$$

Quite clearly, the single-layer contributions are defined as

$$\widetilde{\sigma}^{p}_{\mu\mu}(\varepsilon_1,\varepsilon_2) = \tag{131}$$
$$= \frac{C}{n}\sum_{\alpha=A,B} c_p^\alpha\ \left( tr\left\{\underline{\widetilde{J}}^{p\alpha}_\mu(\varepsilon_2,\varepsilon_1)\underline{\widehat{\tau}}^{pp}_c(\varepsilon_1)\underline{J}^{p\alpha}_\mu(\varepsilon_1,\varepsilon_2)\underline{\widehat{\tau}}^{pp}_c(\varepsilon_2)\right\}\right.$$
$$\left. - \sum_{\beta=A,B} c_p^\beta\, tr\left\{\underline{\widetilde{J}}^{p\alpha}_\mu(\varepsilon_2,\varepsilon_1)\underline{\widehat{\tau}}^{pp}_c(\varepsilon_1)\underline{\widetilde{J}}^{p\beta}_\mu(\varepsilon_1,\varepsilon_2)\underline{\widehat{\tau}}^{pp}_c(\varepsilon_2)\right\}\right)$$

and the layer-layer terms as

$$\widetilde{\sigma}^{pq}_{\mu\mu}(\varepsilon_1,\varepsilon_2) = \tag{132}$$
$$= \frac{C}{n\Omega_{SBZ}}\sum_{\alpha,\beta=A,B} c_p^\alpha c_q^\beta \int tr\left\{\underline{\widetilde{J}}^{p\alpha}_\mu(\varepsilon_2,\varepsilon_1)\underline{\widehat{\tau}}^{pq}_c(\vec{k},\varepsilon_1)\underline{\widetilde{J}}^{q\beta}_\mu(\varepsilon_1,\varepsilon_2)\underline{\widehat{\tau}}^{qp}_c(\vec{k},\varepsilon_2)\right\} d^2k\ .$$

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