1 Schematical view of transport theories

In the following some of the present methods [1] of describing electric transport in solid matter are shortly characterized. The main emphasis of this chapter will be put on the Kubo-Greenwood approach.

1.1 Linearized Boltzmann equation

Assuming for matters of simplicity a cubic system (statistically disordered) then the conductivity tensor is given within the linearized Boltzmann equation as

$$\sigma_{\mu\mu} = \rho_{\mu\mu}^{-1} = \frac{2}{3\hbar}\frac{e^2}{8\pi^3}\int\limits_{E_F} \underbrace{v^{\mu}(k_F)\tau^{B}(k_F)}_{l(k_F)}\, dS_{k_F} \qquad ;$$

$$\mu \in (x, y, z) \qquad ,$$

where

$\sigma_{\mu\mu}$	$\mu\mu$-element of the conductivity tensor
$\rho_{\mu\mu}$	$\mu\mu$-element of the resistivity tensor
$v^{\mu}(k_F)$	μ-like element of the Fermi velocity
$\tau^{B}(k_F)$	relaxation time
$l(k_F)$	mean free path
dS_{k_F}	element of the Fermi surface

Advantage: Easy implementation within traditional band-structure methods, since in the classical interpretation the velocity is given by the energyband dispersion.
Disadvantage: "semi-classical theory", bulk-only, existence of a Fermi surface supposed, $\tau^B(k_F)$ parameters.

1.2 Landauer-Büttiker approach

$$I = \frac{2}{e\hbar}\overline{T}[\mu_1 - \mu_2]$$

$$I_p = \frac{2}{e\hbar}\sum_q \left[\overline{T}_{q\leftarrow p}\mu_p - \overline{T}_{p\leftarrow q}\mu_q\right]$$

μ_1, μ_2	chemical potentials of reservoirs
p, q	terminal end-points
$\overline{T}$	averaged probability for an electron injected at one end-point and transmitted at another

Advantage: Easy classical interpretation for perpendicular transport
Disadvantage: summation over all end-points (also contacts)

1.3 The Kubo equation

Let $\mathbf{H}_0$ be the unperturbed Hamiltonian and $\mathbf{W}(t)$ a time-dependent perturbation. The mean-value of any arbitrary observable can then be described in terms of the equation of motion for the probability operator $\boldsymbol{\rho}(t)$

$$i\hbar\boldsymbol{\rho}(t) = [\mathbf{H}_0 + \mathbf{W}(t), \boldsymbol{\rho}(t)] \quad . \tag{1}$$

In the interaction picture,

$$i\hbar\frac{d}{dt}\boldsymbol{\rho}_{I_W}(t) = \left[\mathbf{W}_{I_W}, \boldsymbol{\rho}_{I_W}\right] \quad , \tag{2}$$

the last equation can be written as a integral equation. Restricting the evaluation to linear terms in $\mathbf{W}_{I_W}$ one gets

$$\boldsymbol{\rho}_{I_W}(t) \approx \boldsymbol{\rho}_{I_W}^{(1)}(t) = \boldsymbol{\rho}_0 - \frac{i}{\hbar}\int_{-\infty}^{t} dt' \left[\mathbf{W}_{I_W}(t')\,\boldsymbol{\rho}_0\right] \quad , \tag{3}$$

where $\boldsymbol{\rho}_0$ is the equilibrium density operator of the canonical ensemble:

$$\boldsymbol{\rho}_0 = \frac{1}{Z}e^{-\beta\mathbf{H}_0}, \tag{4}$$

and

$$Z = Tr\left(e^{-\beta\mathbf{H}_0}\right) \quad , \quad \beta = 1/kT \quad .$$

The average of an operator can now be expressed as

$$\begin{aligned} \langle \mathbf{A} \rangle (t) &= Tr \left(\mathbf{A}_{I_W}(t), \boldsymbol{\rho}_{I_W}(t) \right) && (5) \\ &= \langle \mathbf{A} \rangle_0 - \frac{i}{\hbar} \int_{-\infty}^{t} dt' \, \langle [\mathbf{A}_{I_W}(t), \mathbf{W}_{I_W}(t')] \rangle && (6) \end{aligned}$$

where $\langle \mathbf{A} \rangle_0$ is an average in equilibrium. Assuming that the external perturbation is of the form

$$\mathbf{W}(t) = -\mathbf{B} F(t) \quad ,$$

where $\mathbf{B}$ is a time-independent operator, one gets

$$\langle \mathbf{A} \rangle (t) = \langle \mathbf{A} \rangle_0 - \int_{-\infty}^{\infty} dt' \chi_{AB}(t, t') F(t') \quad , \qquad (7)$$

$\chi_{AB}(t, t')$ being a so-called generalized susceptibility

$$\chi_{AB}(t, t') = \frac{i}{\hbar} \langle [\mathbf{A}_{I_W}(t), \mathbf{B}_{I_W}(t')] \rangle \, \boldsymbol{\Theta}(t - t') \quad , \qquad (8)$$

which in turn can be reformulated as

$$\chi_{AB}(t - t') = \int_0^{\beta} d\lambda \left\langle \frac{d\mathbf{B}}{dt}(t' - i\hbar\lambda) \, \mathbf{A}(t) \right\rangle \boldsymbol{\Theta}(t - t') \, . \qquad (9)$$

Specifying the perturbation as

$$\mathbf{W}(t) = -\mathbf{p}.\mathbf{E}(t) \quad ,$$

and treating the electric field as a periodic quantity,

$$\mathbf{E}_{\omega}\,(t) = \mathbf{E}_0\, e^{-i(\omega+i\delta)t}, \qquad \delta \to 0 \tag{10}$$

one can show that in the indicated case of $\delta \to 0$ (perturbation vanishes at $t = -\infty$) one gets the Kubo formula for the electric conductivity

$$\sigma_{\mu\nu}\,(\omega, T) \;=\; \frac{1}{V}\int_0^{\infty} dt e^{-i\omega t}\int_0^{\beta=1/kT} d\lambda\,\langle J^{\nu}\,(-i\hbar\lambda)\,J^{\mu}\,(t)\rangle \tag{11}$$

$$J\,(t) = e^{iH_0 t/\hbar} J e^{-iH_0 t/\hbar} \quad , \tag{12}$$

where V is the characteristic volume (unit volume) and $J\,(t)$ is the electric current operator.

1.4 The Kubo- and Kubo-Greenwood equation

We will now assume that (1) we can use an effective one-electron picture, (2) the Born-Oppenheimer approximation, and (3) we can form properly the limit of $\omega \rightarrow 0$, then the Kubo equation reduces at $T = 0$ to

$$\sigma_{\mu\mu} = \frac{\pi\hbar}{V} \int_{-\infty}^{\infty} d\epsilon \left(-\frac{\partial f}{\partial \epsilon} \right) \left\langle Tr \left(\delta \left(\epsilon - \mathbf{H} \right) J^{\mu} \delta \left(\epsilon - \mathbf{H} \right) J^{\mu} \right) \right\rangle_{\text{TD}} \tag{13}$$

where f is the Fermi-Dirac distribution function and $\langle\rangle_{\text{TD}}$ denotes a thermodynamical average, which at $T = 0$ can be replaced by an averaged over all configurations of an alloy. Rewritting finally the Dirac δ-functions as

$$\begin{aligned} \delta \left(\epsilon - \mathbf{H} \right) &= -\frac{1}{\pi} \operatorname{Im} \mathbf{G}^{+} \left(\epsilon \right) \\ &= -\frac{1}{2\pi i} \left(\mathbf{G}^{+} \left(\epsilon \right) - \mathbf{G}^{-} \left(\epsilon \right) \right) \\ &= \sum_{n} \left| n \right\rangle \left\langle n \right| \delta \left(\epsilon - \epsilon_{n} \right) \quad , \end{aligned} \tag{14}$$

the **diagonal components** of the conductivity tensor

$$\sigma_{\mu\mu} = \frac{\pi\hbar}{V} \left\langle \sum_{mn} J^{\mu}_{mn} J^{\mu}_{nm} \delta\left(\epsilon_F - \epsilon_m\right) \delta\left(\epsilon_F - \epsilon_n\right) \right\rangle_{\text{conf.}} \quad , \tag{15}$$

are given by

$$\sigma_{\mu\mu} \; = \; \frac{\hbar}{\pi V} \left\langle Tr \left(J^{\mu} \operatorname{Im} \mathbf{G}^{+}\left(\epsilon_{\mathrm{F}}\right) J^{\mu} \operatorname{Im} \mathbf{G}^{+}\left(\epsilon_{\mathrm{F}}\right) \right) \right\rangle_{\text{conf.}} \tag{16}$$

$$\mu \; \in \; \{x, y, z\} \quad , \tag{17}$$

where the J^{μ}_{mn} are the matrix elements of the current operator in the basis $\{|n\rangle\}$.

The **off-diagonal components** require a more complicated integration path in the complex plane, see [8]

2 Applications of the Kubo-Greenwood approach to layered systems

2.1 General expressions

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

$$\sigma_{\mu\nu} = \frac{\pi\hbar}{N_0\Omega_{at}} \left\langle \sum_{m,n} J^{\mu}_{mn} J^{\nu}_{nm} \delta(\epsilon_F - \epsilon_m)\delta(\epsilon_F - \epsilon_n) \right\rangle \quad . \tag{18}$$

In this equation $\mu, \nu \in \{x, y, z\}$, N_0 is the number of atoms, J^{ν} is a representation of the ν-th component of the current operator,

$$J^{\nu} = \{J^{\nu}_{nm}\} \quad ; \quad J^{\nu}_{nm} = \langle n \mid J_{\nu} \mid m \rangle \quad , \tag{19}$$

$\mid m\rangle$ is an eigenstate of a particular configuration of the random system, Ω_{at} is the atomic volume, and $\langle \cdots \rangle$ denotes an average over configurations. Eq. (18) can be reformulated in terms of the imaginary part of the (one-particle) Green's function

$$\sigma_{\mu\nu} = \frac{\hbar}{\pi N_0 \Omega_{at}} Tr \ \left\langle J_\mu Im G^+(\epsilon_F) J_\nu Im G^+(\epsilon_F) \right\rangle \quad . \quad (20)$$

or by using ”up-” and ”down-” side limits, this equation can be rewritten as

$$\sigma_{\mu\nu} \ = \ \frac{1}{4} \left\{ \widetilde{\sigma}_{\mu\nu}(\epsilon^+, \epsilon^+) + \widetilde{\sigma}_{\mu\nu}(\epsilon^-, \epsilon^-) \right. \quad (21)$$

$$\left. - \widetilde{\sigma}_{\mu\nu}(\epsilon^+, \epsilon^-) - \widetilde{\sigma}_{\mu\nu}(\epsilon^-, \epsilon^+) \right\} \quad ,$$

where

$$\epsilon^+ = \epsilon_F + i\delta \quad , \quad \epsilon^- = \epsilon_F - i\delta \quad ; \quad \delta \to 0 \quad ,$$

and

$$\widetilde{\sigma}_{\mu\nu}(\epsilon_1, \epsilon_2) \ = \ -\frac{\hbar}{\pi N_0 \Omega_{at}} tr \ \left\langle J_\mu G(\epsilon_1) J_\nu G(\epsilon_2) \right\rangle \quad ; \ (22)$$

$$\epsilon_i \ = \ \epsilon^\pm \quad ; \quad i = 1, 2 \quad .$$

<u>Scattering theory:</u>

$$G(z) \Rightarrow \tau(z)$$

where $\tau(z)$ is the so-called scattering path operator.

2.2 Conductivity for layered systems

As in the bulk case a typical contribution to the conductivity can be expressed in terms of real space scattering path operators,

$$\widetilde{\sigma}_{\mu\nu}(\epsilon_1, \epsilon_2) \tag{23}$$

$$= (C/N_0) \sum_{p=1}^{n} \left\{ \left\{ \sum_{i \in I(L_2)} \sum_{q=1}^{n} \right.\right.$$

$$\left.\left. \sum_{j \in I(L_2)} tr \left\langle J_\mu^{pi}(\epsilon_2, \epsilon_1) \tau^{pi,qj}(\epsilon_1) J_\nu^{qj}(\epsilon_1, \epsilon_2) \tau^{qj,pi}(\epsilon_2) \right\rangle \right\} \right\}$$

where $C = -\left(4m^2/\hbar^3 \pi \Omega_{at}\right)$ and $N_0 = nN$ is the total number of sites in the intermediate region (multilayer), as given in terms of the number of layers in the multilayer (n) and the order of the two-dimensional translational group N (number of atoms in one layer).

2.3 Current matrices

Let $J_{\mu}^{p\alpha}(\epsilon_1, \epsilon_2)$ 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 $\mathbf{J} = (e\hbar/im)\,\boldsymbol{\nabla}$, the elements of $J_{\mu}^{p\alpha}(\epsilon_1, \epsilon_2)$ are given by

$$J_{\mu,\Lambda\Lambda'}^{p\alpha}(\epsilon_1, \epsilon_2) = \frac{e}{m}\frac{\hbar}{i}\int\limits_{WS} Z_{\Lambda}^{p\alpha}(\mathbf{r}_{p0}, \epsilon_1)^{\dagger}\frac{\partial}{\partial r_{p0,\mu}} Z_{\Lambda'}^{p\alpha}(\mathbf{r}_{p0}, \epsilon_2) d^3 r_{p0} \tag{24}$$

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

$$J_{\mu,\Lambda\Lambda'}^{p\alpha}(\epsilon_1, \epsilon_2) = ec\int\limits_{WS} Z_{\Lambda}^{p\alpha}(\mathbf{r}_{p0}, \epsilon_1)^{\dagger}\alpha_{\mu} Z_{\Lambda'}^{p\alpha}(\mathbf{r}_{p0}, \epsilon_2) d^3 r_{p0} \quad . \tag{25}$$

In Eqs. (24), (25) the functions $Z_{\Lambda}^{p\alpha}(\mathbf{r}_{p0}, z)$ are the usual scattering solutions.

2.4 Two-dimensional translational symmetry

Assuming two-dimensional invariance applies in all layers under consideration, a typical contribution $\widetilde{\sigma}_{\mu\nu}(\epsilon_1, \epsilon_2)$ to the conductivity is therefore given by

$$\widetilde{\sigma}_{\mu\nu}(\epsilon_1, \epsilon_2) \tag{26}$$

$$= (C/n) \sum_{p=1}^{n} \sum_{q=1}^{n}$$

$$\left\{ \sum_{j \in I(L_2)} tr \left\langle J_\mu^{p0}(\epsilon_2, \epsilon_1) \tau^{p0,qj}(\epsilon_1) J_\nu^{qj}(\epsilon_1, \epsilon_2) \tau^{qj,p0}(\epsilon_2) \right\rangle \right\} \quad ,$$

where $p0$ specifies the origin of L_2 for the p-th layer.

2.5 Vertex corrections for the average of the product of two single-particle GF's

$$\left\langle J_\mu^{p0}(\epsilon_2,\epsilon_1)\tau^{p0,qj}(\epsilon_1)J_\nu^{qj}(\epsilon_1,\epsilon_2)\tau^{qj,p0}(\epsilon_2)\right\rangle$$

$$= \left\langle J_\mu^{p0}(\epsilon_2,\epsilon_1)\tau^{p0,qj}(\epsilon_1)\right\rangle (1-\Omega)\left\langle J_\nu^{qj}(\epsilon_1,\epsilon_2)\tau^{qj,p0}(\epsilon_2)\right\rangle$$

Omitting vertex corrections $(\Omega = 0)$, one gets

$$\left\langle J_\mu^{p0}(\epsilon_2,\epsilon_1)\tau^{p0,qj}(\epsilon_1)J_\nu^{qj}(\epsilon_1,\epsilon_2)\tau^{qj,p0}(\epsilon_2)\right\rangle$$

$$= J_\mu^{p0}(\epsilon_2,\epsilon_1)\left\langle \tau^{p0,qj}(\epsilon_1)\right\rangle J_\nu^{qj}(\epsilon_1,\epsilon_2)\left\langle \tau^{qj,p0}(\epsilon_2)\right\rangle$$

Note that

$$\left\langle J_\mu^{p0}(\epsilon_2,\epsilon_1)\right\rangle = J_\mu^{p0}(\epsilon_2,\epsilon_1)$$

(two-dimensional invariance).

2.6 Coherent Potential Approximation

From the inhomogeneous CPA condition (single site approximation, no fluctuation terms!) for a binary disordered layered system (constituents A and B),

$$\widehat{\tau}_c^{pp}(z) = \sum_{\alpha=A,B} c_p^\alpha \left\langle \widehat{\tau}^{pp}(z) \right\rangle_{p,\alpha} \quad , \tag{27}$$

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

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

where the so-called impurity matrix is then given by

$$\widehat{D}_\alpha^{pp}(z) \equiv D_\alpha^{p0,p0}(z) = \left[1 - m_\alpha^p(z) \tau_c^{p0,p0}(z)\right]^{-1} \quad , \tag{28}$$

$$m_\alpha^p(z) = t_c^p(z)^{-1} - t_\alpha^p(z)^{-1}, \quad \alpha = A, B \quad ,$$

and $t_\alpha^p(z)$ is the single–site t–matrix for constituent α in layer p, follows .

$$\left\langle \widehat{\tau}^{pp}(z) \right\rangle_{p,\alpha} \equiv \left\langle \tau^{p0,p0}(z) \right\rangle_{p0,\alpha} \tag{29}$$

$$= \left\langle \tau^{pi,pi}(z) \right\rangle_{pi,\alpha} \quad , \quad \forall i \in I(L_2) \quad ,$$

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

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

$$p \neq q, \quad \forall i,j \in I(L_2) \quad : \tag{30}$$

$$\left\langle \tau^{pi,qj}(z) \right\rangle_{pi\alpha,qj\beta} = \widehat{D}^{pp}_{\alpha}(z)\tau^{pi,qj}_{c}(z)\widehat{D}^{qq}_{\beta}(z)^{t} \quad ,$$

$$p = q: \quad \forall (i \neq j) \in I(L_2) \quad : \tag{31}$$

$$\left\langle \tau^{pi,pj}(z) \right\rangle_{pi\alpha,pj\beta} = \widehat{D}^{pp}_{\alpha}(z)\tau^{pi,pj}_{c}(z)\widehat{D}^{pp}_{\beta}(z)^{t} \quad ,$$

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

2.7 Total conductivity for layered systems

Using the $\Omega = 0$ approximation and the (inhomogeneous) Coherent Potential Approximation, a typical contribution

$$\widetilde{\sigma}_{\mu\nu}(\epsilon_1, \epsilon_2)$$

to the conductivity is then given by

$$\widetilde{\sigma}_{\mu\nu}(\epsilon_1, \epsilon_2) = (C/n)\times$$

$$\sum_{p=1}^{n} \left\{ \sum_{\alpha=A,B} c_p^\alpha tr \left[\widetilde{J}_\mu^{p\alpha}(\epsilon_2, \epsilon_1) \widehat{\tau}_c^{pp}(\epsilon_1) J_\nu^{p\alpha}(\epsilon_1, \epsilon_2) \widehat{\tau}_c^{pp}(\epsilon_2) \right] \right.$$

$$- \sum_{\alpha,\beta=A,B} c_p^\alpha c_p^\beta tr \left[\widetilde{J}_\mu^{p\alpha}(\epsilon_2, \epsilon_1) \widehat{\tau}_c^{pp}(\epsilon_1) \widetilde{J}_\nu^{p\beta}(\epsilon_1, \epsilon_2) \widehat{\tau}_c^{pp}(\epsilon_2) \right]$$

$$+ \Omega_{SBZ}^{-1} \sum_{q=1}^{n} \sum_{\alpha,\beta=A,B} c_p^\alpha c_q^\beta \times$$

$$\left. \times\, tr \int \left[\widetilde{J}_\mu^{p\alpha}(\epsilon_2, \epsilon_1) \widehat{\tau}_c^{pq}(\mathbf{k}, \epsilon_1) \widetilde{J}_\nu^{q\beta}(\epsilon_1, \epsilon_2) \widehat{\tau}_c^{qp}(\mathbf{k}, \epsilon_2) d^2k \right] \right\} \tag{32}$$

where

$$\widetilde{J}_{\mu}^{p\alpha}(\epsilon_2,\epsilon_1) = \widehat{D}_{\alpha}^{pp}(\epsilon_2)^t J_{\mu}^{p\alpha}(\epsilon_2,\epsilon_1)\widehat{D}_{\alpha}^{pp}(\epsilon_1) \tag{33}$$

As one can see one such conductivity contribution contains layer-diagonal and layer-off-diagonal terms, whereby the computationally expensive part is hidden in the integration over the surface Brillouin zone.

[1] S. Datta, *Electronic Transport in Mesoscopic Systems*, Cambridge University Press, 1995

[2] J. M. Luttinger, *Transport Theory*, in *Mathematical Methods in Solid State and Superfluid Theory*, Eds. R. C. Clark and G. H. Derrick (Oliver & Boyd, Edinburgh, 1967) pp. 157-193.

[3] J. Banhart, *Transporteigenschaften komplexer metallischer Systeme*, Habilitation, 1997.

[4] L. Smrka and P. Steda, J. Phys.C.: Solid State Phys. **10**, 2153 (1977).

[5] W. H. Butler, Phys. Rev. B **31**, 3260 (1985).

[6] X.-G. Zhang and W. H. Butler, Phys. Rev. B **55**, 10 308 (1997).

[7] P. Weinberger, P.M. Levy, J. Banhart, L. Szunyogh, and B. Újfalussy, J. Phys.: Condens. Matter **8**, 7679 (1996).

[8] L. Szunyogh and P. Weinberger, J. Phys. Cond. Matt. **11**, 10 451 (1999).