1 The Kubo-Greenwood equation

Within the Kubo-Greenwood formulation the (diagonal) elements of the electric conductivity tensor are given by

$$\sigma^{\mu\mu} = \frac{\hbar}{\pi N_0 \Omega_{at}} Tr \left\langle J^\mu Im G^+(\epsilon_F) J^\mu Im G^+(\epsilon_F) \right\rangle \quad (1)$$

$$\mu \in (x, y, z) \quad (2)$$

where N_0 is the total number of atoms, Ω_{at} the atomic volume, J^μ the current operator and $G^+(\epsilon_F)$ the one-particle resolvent.

Using multiple sacttering for systems with only two-dimensional translational symmetry (semi-infinite systems) $\sigma^{\mu\mu}$ can be written in terms of "two-point" condictivities $\sigma^{\mu\mu}$

$$\sigma^{\mu\mu}(n) = \sum_{i,j=1}^{n} \sigma_{ij}^{\mu\mu}(n) \quad , \quad (3)$$

with i and j denoting planes of atoms and n the total number of planes.

2 System characterization

boundary conditions	metal layers	spacer layers	metal layers	boundary conditions
■	⊛	⊡	⊛	■
■	⊛	⊡	⊛	■
■	⊛	⊡	⊛	■
■	⊛	⊡	⊛	■

$\mathcal{M} = \{\mathbf{M}_i \mid i \in \mathbb{N}^+\}$	Orientations of the magnetization
$\mathcal{J} = \{\mathbf{j}_i \mid i \in \mathbb{N}^+\}$	directions of the current

3 Mapping

In the following for CPP the (two-point-) conductivity tensor $\sigma(z, z')$, where z and z' are contineous variables along the growth ($\widehat{z}$-) direction, is mapped onto the conductivity tensor for a layered system, $\sigma_{ij}^{zz}(n) \equiv \sigma_{ij}(n), i, j = 1, n$, such that the algebraic structure as defined below is conserved:

$$\boxed{\begin{array}{l} \sigma(z,z') \\ \\ \int \rho(z,z'')\sigma(z'',z') \\ \qquad = \delta(z-z') \end{array}}$$

$$\searrow g : \quad \boxed{r = \iint \rho(z,z')dzdz'}$$

$$\downarrow f : \qquad \nearrow g' : \quad \boxed{r(n) = \sum_{i,j=1}^{n} \rho_{ij}(n)}$$

$$\boxed{\begin{array}{l} \sigma_{ij}(n) \\ \\ \sum_k \rho_{ik}(n)\sigma_{kj}(n) = \delta_{ij} \end{array}}$$

$$\begin{array}{l} f : \sigma(z,z') \longrightarrow \sigma_{ij}(n) \\ g : \rho(z,z') \longrightarrow r \\ g' : \rho_{ik}(n) \ \longrightarrow r(n) \end{array}$$

Clearly enough the sheet resistance then serves as measure for the mapping, since according to the Cauchy convergence criterion the integral in here can be replaced by a sum if and only if,

$$\left| r - \lim_{n\to\infty} r(n) \right| < \Delta \quad , n \in \mathbb{N}^+ \quad , \tag{4}$$

or

$$|r(n+m) - r(n)| < \Delta; \qquad n, m \in \mathbb{N}^+ \quad , \tag{5}$$

where Δ is an infinitesimal small number.

4 Current conservation

In a layered system the current (in the direction of the surface normal, CPP) with respect to a particular layer i is given by

$$j_i(n) = \sum_{j=1}^{n} \sigma_{ij}(n) E_j(n) \tag{6}$$

$$\sum_{j=1}^{n} \rho_{ij}(n) \sigma_{jk}(n) = \delta_{ik} \qquad , \tag{7}$$

where the $E_j(n)$ are the layer-resolved $z-$components of the electric fields. Using this equation in the following manner

$$\rho_{ki}(n) j_i(n) = \rho_{ki}(n) \sum_{j} \sigma_{ij} E_j(n) \qquad , \tag{8}$$

$$\sum_{i} \rho_{ki}(n) j_i(n) = \sum_{j} \underbrace{\sum_{i} \rho_{ki}(n) \sigma_{ij}(n)}_{=\delta_{kj}} E_j(n) = E_k(n) \tag{9}$$

one gets

$$\sum_{k,i=1}^{n} \rho_{ki}(n) j_i(n) = \sum_{k} E_k(n) \equiv E_0(n) \qquad . \tag{10}$$

Under steady-state conditions (**current conservation**), i.e., $j_i(n) = j_0, \forall i, n$, then

$$j_0 \left[\sum_{k,i=1}^{n} \rho_{ki}(n) \right] = j_0 r(n) = E_0(n) \qquad , \qquad (11)$$

where

$$r(n) = \sum_{i,j=1}^{n} \rho_{ij}(n) \qquad , \qquad (12)$$

which again leads to the Cauchy relations

$$\begin{aligned} |E_0(n+m) - E_0(n)| &\leq \Delta \qquad (13) \\ &\looparrowright |r(n+m) - r(n)| \leq \Delta \\ n, m &\in \mathbb{N}^+ \end{aligned}$$

5 Layer-resolved sheet resistances and complex energies

Layer-resolved sheet resistances $r_i(n)$ can be defined

$$r_i(n) = \sum_{j=1}^{n} \rho_{ij}(n) \quad , \tag{14}$$

such that

$$r(n) = \sum_{i=1}^{n} r_i(n) \quad . \tag{15}$$

Suppose $\mathcal{C}$ denotes a particular magnetic configuration (a set of classical unit vectors characterizing the orientations of the magnetization in each layer of the system) and δ is the imaginary part of the complex Fermi energy $\epsilon_F + i\delta$ then

$$r(\mathcal{C}; n) = \lim_{\delta \to 0} r(\mathcal{C}; n; \delta) = \lim_{\delta \to 0} \sum_{i,j=1}^{n} \rho_{ij}(\mathcal{C}; n; \delta) \quad , \tag{16}$$

where

$$\sum_{k=1}^{n} \rho_{ik}(\mathcal{C}; n; \delta) \sigma_{kj}(\mathcal{C}; n; \delta) = \delta_{ij} \quad . \tag{17}$$

6 Pure metals or leads:

6.1 Layer-dependence:

For a large enough n $(n \geq n_0)$ and a given imaginary part δ of the complex Fermi energy $\epsilon_F + i\delta$,the corresponding sheet resistance $r(\mathcal{C}; n; \delta)$ varies linearly with n,

$$k_1(\mathcal{C}; \delta) = \frac{r(\mathcal{C}; n+m; \delta) - r(\mathcal{C}; n; \delta)}{m} \quad ; \quad m \in \mathbb{N}^+ \quad , \tag{18}$$

i.e., the following relation applies

$$r(\mathcal{C}; n; \delta) = r_0(\mathcal{C}; \delta) + n k_1(\mathcal{C}; \delta) \quad , \tag{19}$$

with $r_0(\mathcal{C}; \delta)$ being the value for the linear behavior defined by eqn. (18) at $n = 0$.

6.2 Dependence on the imaginary part of the Fermi energy

$r(\mathcal{C}; n, \delta)$ also varies linearly in δ:

$$k_2(\mathcal{C}; n) = \frac{1}{n} \frac{r(\mathcal{C}; n; \delta_2) - r(\mathcal{C}; n; \delta_1)}{\Delta} \quad , \quad \Delta = \delta_2 - \delta_1 \quad , \tag{20}$$

i.e.,

$$r(\mathcal{C};n;\delta) = r_0(\mathcal{C};n) + n\delta k_2(\mathcal{C};n) \quad , \tag{21}$$

where as will become clear in a moment the constant $k_2(\mathcal{C};n)$ is chosen to be normalized per layer and $k_2(\mathcal{C};n)$ follows the below behavior,

$$\lim_{\delta\to 0} k_2(\mathcal{C};n) = 0 \quad . \tag{22}$$

6.3 Combined dependence

Combining now eqn (19) with eqn. (21),

$$r_0(\mathcal{C};\delta) + nk_1(\mathcal{C};\delta) = r_0(\mathcal{C};n) + n\delta k_2(\mathcal{C};n) \quad , \tag{23}$$

one gets

$$r_0(\mathcal{C};\delta) = r_0(\mathcal{C};n) + n\Phi(\delta) \quad , \tag{24}$$

where

$$\Phi(\delta) = \delta k_2(\mathcal{C};n) - k_1(\mathcal{C};\delta) \quad . \tag{25}$$

Demanding that

$$r_0(\mathcal{C};n) = \lim_{\delta\to 0} r_0(\mathcal{C};\delta) \quad , \tag{26}$$

requires that

$$\lim_{\delta\to 0} \Phi(\delta) = 0 \quad , \tag{27}$$

which in in turn implies that

$$\boxed{\lim_{\delta\to 0} k_1(\mathcal{C};\delta) = 0} \tag{28}$$

since $\delta k_2(\mathcal{C};n)$ trivially vanishes for $\delta \to 0$.

6.4 Resistivity and boundary condition at n$\to \infty$

From eqns. (18) and (26) follows that for $n \geq n_0$

$$\lim_{\delta\to 0} r(\mathcal{C};n+m;\delta) = r_0(\mathcal{C};n) \equiv r_0(\mathcal{C}); m \in \mathbb{N}^+ \quad , \tag{29}$$

which, however, is nothing but the Cauchy convergence criterion for the sheet resistance demanded in eqn. (5):

$$\lim_{\delta\to 0} [r(\mathcal{C};n+m;\delta) - r(\mathcal{C};n;\delta)] = 0 \quad .$$

Quite clearly since $r_0(\mathcal{C})$ is a constant for a pure metal this leads to a correct bulk resistivity $\rho_{zz}^{bulk}(\mathcal{C})$,

$$\rho_{zz}^{bulk}(\mathcal{C}) = \lim_{n\to\infty} \left[\frac{r_0(\mathcal{C})}{L}\right] = \frac{1}{d} r_0(\mathcal{C}) \lim_{n\to\infty} \frac{1}{n} = 0 \quad ,$$

where d is the interplanar distance.

7 Heterojunctions: .../$\mathbf{L}_n\mathbf{X}_m\mathbf{L}_n$/...

For $n \geq n_0$ the sheet resistance $r(\mathcal{C}; 2n+s; \delta)$ for a given value of δ varies linear with respect to n,

$$k_1(\mathcal{C};\delta) = \frac{r(\mathcal{C}; 2(n+m)+s; \delta) - r(\mathcal{C}; 2n+s; \delta)}{2m}, \tag{30}$$

$$m \geq 0 \in \mathbb{N}^+ \tag{31}$$

i.e.,

$$r(\mathcal{C}; 2(n+m)+s; \delta) = r(\mathcal{C}; 2n \geq +s; \delta) - 2mk_1(\mathcal{C};\delta) \tag{32}$$

The relevant part of the heterojunction is therefore defined by the condition that for $n \geq n_0$ the sheet resistance starts to grow linear in n, i.e.,

$$r(\mathcal{C}; 2n_0+s) = \lim_{\delta \to 0} r(\mathcal{C}; 2n_0+s; \delta) \tag{33}$$

With $L = (2n_0+s)\, a_0/2$ one gets the corresponding resistivity

$$\rho(\mathcal{C}; 2n_0+s) = \frac{2}{(2n_0+s)\, a_0} \lim_{\delta \to 0} r(\mathcal{C}; 2n_0+s; \delta) \tag{34}$$

$$= \frac{2}{(2n_0 + s)\, a_0} r(\mathcal{C}; 2n_0 + s)$$

The magnetoresistance is then given as

$$R(2n_0 + s) = \frac{r(\mathcal{AP}; 2n_0 + s) - r(\mathcal{P}; 2n_0 + s)}{r(\mathcal{AP}; 2n_0 + s)} \tag{35}$$

or approximatively by

$$R(2n_0 + s; \delta) = \frac{r(\mathcal{AP}; 2n_0 + s; \delta) - r(\mathcal{P}; 2n_0 + s; \delta)}{r(\mathcal{AP}; 2n_0 + s; \delta)} \tag{36}$$

It should be noted that since $R(\delta) \leq R$ this quantity can be used for qualitative discussions of the magnetoresistance.

8 Definitions:

ρ_{xx}	**in-plane** <u>resistivity</u>
ρ_{zz}	**perpendicular** <u>resistivity</u>
L	**length**
$L\rho_{zz}$	<u>sheet resistance</u>
$L^2\rho_{zz}$	<u>resistance</u>