Relativistic and non-relativistic electron transport in disordered alloys: I. Theory [1]

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Abstract

The electrical conductivity of disordered alloys is calculated using the Korringa-Kohn-Rostoker–coherent potential approximation (KKR–CPA) alloy theory in conjunction with the local approximation to density functional theory and the Kubo-Greenwood equation. Relativistic and non-relativistic expressions for the conductivity are derived. A technique for the evaluation of the Kubo-Greenwood equation for arbitrary crystal symmetry using group theoretical methods is described. Explicit expressions for scattering and current operators at complex energies below the real axis which occur in the evaluation of the Kubo-Greenwood equation are given.

1 Introduction

Describing and calculating transport properties of metallic systems is a task of considerable complexity and is much more challenging than the calculation of thermodynamic equilibrium observables. The reason for this is that transport processes imply the usage of irreversible thermodynamics and therefore complicate the treatment of such phenomena a lot (Doniach and Sondheimer 1974; Rickayzen 1980; Mahan 1981; Kubo, Toda and Hashitsume 1985). In principle there are two methods for calculating transport properties of metallic systems: either by solving a kinetic equation such as the semiclassical Boltzmann equation (Ziman 1967) or by applying linear-response theory (Kubo 1957). The former approach is limited to cases where the mean free path of the electrons is large in comparison to the lattice spacing and therefore to cases of weak or modest disorder. The latter approach has the advantage of being free of such limitations allowing for a treatment of strongly disordered systems where the mean free path is very short. However, the kinetic equations permit the treatment of non-linear response whereas by definition this is not possible in the framework of linear-response theory. The two approaches lead to identical results in the limit of weak scattering and weak external fields (Edwards 1958; Schotte 1978; Mahan 1987).

[1] Published in: Philosophical Magazine B 77(1), 85—103 (1998)

The electrical resistivity of disordered alloys is one of the most impressive manifestations of disorder. At zero temperature the resistivity of a pure metal or an ordered alloy vanishes, whereas disordered alloys have resistivities which can be as high as 200 $\mu\Omega$·cm in some cases. Because the electrical resistivity of normal metals and alloys is a linear phenomenon — Ohm's law is valid — linear-response theory is the adequate tool for treating such systems.

The electronic structure of disordered alloys can be described very efficiently in the framework of a local approximation to density functional theory and by means of the coherent-potential approximation (CPA) which gives an accurate description of the disordered state (Ehrenreich and Schwartz 1976; Faulkner 1982; Gonis 1992). In particular, applying the CPA in conjunction with the Korringa-Kohn-Rostoker (KKR) band theory allows for a first-principles treatment of such alloys (Weinberger 1990; Gonis 1992). The KKR–CPA yields a configuration-averaged Green function which can be used for linear-response transport theory by inserting it into the Kubo-Greenwood equation (Kubo 1957; Greenwood 1958). Butler showed how to perform the configurational average required in the evaluation of the Kubo-Greenwood equation for disordered systems in the framework of the KKR–CPA (Butler 1985) by following the ideas of Velický (1969). Applications of the formalism to various alloy systems demonstrated that this theory allows for a parameter-free first-principles treatment of transport quantities and yields numerical results which are in good agreement with experimental findings (Swihart, Butler, Stocks, Nicholson and Ward 1986; Brown, Allen, Nicholson and Butler 1989; Banhart, Ebert and Weinberger 1994; Banhart and Ebert 1995). Quite recently the Kubo-Greenwood formalism has been extended to deal with layered systems such as magnetic multilayer systems which show the GMR effect (Weinberger, Levy, Banhart, Szunyogh and Újfalussy 1996). It is the purpose of the present and a following paper (Banhart 1997) to carry on the existing work on the application of the Kubo-Greenwood equation to disordered alloys. Relativistic and non-relativistic versions of the theory are presented. For this, expressions for the current operators corresponding to these two cases are derived. An efficient way for the calculation of Brillouin zone averages of products of scattering-path operators using the symmetry properties of the lattice is presented and the matrix structure of such averages discussed. Moreover, simple expressions for the various scattering quantities in the regime of complex energies with negative imaginary parts are given.

2 Kubo-Greenwood equation

Linear-response theory provides very general expressions for transport coefficients which are exact in the limit of weak external fields. The frequency dependent electrical conductivity tensor $\sigma(\omega)$, e.g., can be

written as (Kubo 1957):

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

where V is the volume of the system, and J is the current operator in the unperturbed Heisenberg picture. $\langle \ldots \rangle$ denotes a thermodynamical average. This expression, although very general and exact, is not suitable for practical calculations. However, by making some additional assumptions one can derive an equation which is more useful. In particular one assumes a one-electron picture of the electronic system, considers merely elastic scattering by static impurities and neglects the motion of the ions. The diagonal components of the electrical conductivity tensor of a disordered metallic conductor at zero temperature, i.e., with disorder originating from the atomic arrangement only, can then be written as (Greenwood 1958; Chester and Thellung 1959; Kubo 1959; Verboven 1960; Economou 1983):

$$\sigma_{\mu\mu} = \frac{\pi\hbar}{V} \left\langle \mathrm{Tr}\Big(\delta(\epsilon - \boldsymbol{H})\, J^\mu\, \delta(\epsilon - \boldsymbol{H})\, J^\mu \Big) \right\rangle_{\mathsf{conf.}}, \quad \mu \in \{x, y, z\}. \tag{2}$$

This is one form of the Kubo-Greenwood equation. By using the Green function G of the system which is given by (Economou 1983):

$$\delta(\epsilon - \boldsymbol{H}) = -\frac{1}{\pi} \mathrm{Im}\boldsymbol{G}^+(\epsilon), \tag{3}$$

one obtains an alternative form:

$$\sigma_{\mu\mu} = \frac{\hbar}{\pi V} \left\langle \mathrm{Tr}\Big(J^\mu\, \mathrm{Im}G^+(\epsilon)\, J^\mu\, \mathrm{Im}G^+(\epsilon) \Big) \right\rangle_{\mathsf{conf.}} \tag{4}$$

where J^μ denotes the current operator in the μ-th spatial direction. The average has to be taken over all possible configurations of the disordered system in both cases.

If one introduces the concepts of multiple-scattering theory, one rather uses Green functions than wave functions to describe the electronic structure. The formulation of the KKR–CPA is based on the so-called scattering-path operator τ, which is related to the one-particle Green function by (Faulkner and Stocks 1980):

$$\begin{aligned} G(\vec{r}, \vec{r'}, \epsilon) = \frac{2m_e}{\hbar^2} \sum_{Q,Q'} \Bigg[& Z_Q^m(\vec{r}_m, \epsilon) \boldsymbol{\tau}_{QQ'}^{mn}(\epsilon) Z_{Q'}^{\dagger n}(\vec{r'}_n, \epsilon) \\ & - \Big(Z_Q^m(\vec{r}_m, \epsilon) Z_{i,Q'}^{\dagger n}(\vec{r'}_n, \epsilon)\theta(r' - r) + Z_{i,Q}^m(\vec{r}_m, \epsilon) Z_{Q'}^{\dagger n}(\vec{r'}_n, \epsilon)\theta(r - r') \Big) \delta_{mn}\delta_{QQ'} \Bigg], \end{aligned} \tag{5}$$

where $\vec{r} = \vec{R}_m + \vec{r}_m$, $\vec{r'} = \vec{R}_n + \vec{r'}_n$ and Z and Z_i are regular and irregular solutions of the radial Schrödinger or Dirac equation, respectively. $\theta(r)$ is the usual step function. The angular momentum indices Q may either denote a non-relativistic (e.g. the (ℓ,m$_\ell$)-representation) or a relativistic representation such as the Λ- or γ-representation (Onodera and Okazaki 1966). The Green function is a 4×4 matrix in the relativistic case, a scalar otherwise. As the scattering-path operator contains the same information as the Green function or the wave function, the Kubo-Greenwood equation can be rewritten in terms of this operator yielding:

$$\sigma_{\mu\mu}(\epsilon) = -\frac{m_e^2}{\pi\hbar^3 V} \sum_{z_1,z_2} s_{z_1,z_2} \sum_{mn} \sum_{\substack{Q_1,Q_2 \\ Q_3,Q_4}} \left\langle J^{m\mu}_{Q_4Q_1}(z_2,z_1) \tau^{mn}_{Q_1Q_2}(z_1) J^{n\mu}_{Q_2Q_3}(z_1,z_2) \tau^{nm}_{Q_3Q_4}(z_2) \right\rangle_{\mathsf{conf.}}, \tag{6}$$

where $s_{z_1,z_2} = (2\delta_{z_1,z_2} - 1)$ and z_1, z_2 are the two side limits of the complex energies defined by $z_{1,2} = \epsilon \pm i\eta$, with $\eta \to 0$. The decomposition of Eq. 4 into four terms avoids the explicit occurrence of expressions of the type "Im(G)". $J^{m\mu}$ are the matrix elements of the current operator with respect to the functions Z^m in cell m. Expressions for these matrix elements shall be derived in the next section. Eq. 6 is the starting point for the formulation of the Kubo-Greenwood equation in the framework of the KKR–CPA. Butler showed how to perform the explicit configuration average in Eq. 6 analytically and obtained an expression for the electrical conductivity tensor in terms of KKR-like quantities (Butler 1985):

$$\begin{aligned} \sigma_{\mu\mu} = -\frac{m_e^2}{\pi\hbar^3\Omega} \sum_{z_1,z_2} s_{z_1,z_2} \quad \Big(\quad & \sum_{\alpha,\beta} c^\alpha c^\beta \tilde{J}^{\alpha\mu}(z_2,z_1) \underbrace{\left\{1 - \chi^{\mathsf{CPA}}(z_1,z_2)\omega(z_1,z_2)\right\}^{-1}}_{\mathrm{VC}} \chi^{\mathsf{CPA}}(z_1,z_2) \tilde{J}^{\beta\mu}(z_1,z_2) \\ + \quad & \sum_{\alpha} c^\alpha \, \tilde{J}^{\alpha\mu}(z_2,z_1) \, \tau^{\mathsf{CPA}}(z_1) \, J^{\alpha\mu}(z_1,z_2) \, \tau^{\mathsf{CPA}}(z_2) \Big). \end{aligned} \tag{7}$$

where Ω is the volume of the unit cell. In Eq. 7 angular momentum indices have been omitted for the sake of simplicity. The matrix quantities are to be multiplied in a straightforward way. The scattering operators occurring in this equation are averaged with respect to the CPA medium: the scattering path operator τ^{CPA} is related to the CPA-t-matrix (coherent single-site t-matrix) and the structure constants $G^0(\vec{k})$ by a Brillouin zone integral:

$$\tau^{\mathsf{CPA}}(z) = \frac{1}{\Omega_{\mathsf{BZ}}} \int_{BZ} \tau(\vec{k},z) d^3k \tag{8}$$

with

$$\tau(\vec{k},z) = \left[\left(t^{\mathsf{CPA}}(z) \right)^{-1} - G^0(\vec{k},z) \right]^{-1} \tag{9}$$

and χ^{CPA} is essentially the Brillouin zone average of a pair of operators $\tau(\vec{k}, z)$ defined in Eq. 9:

$$\chi^{\mathsf{CPA}}(z_1, z_2) = \frac{1}{\Omega_{\mathsf{BZ}}} \int_{BZ} \tau(\vec{k}, z_1)\tau(\vec{k}, z_2) d^3k - \tau^{\mathsf{CPA}}(z_1)\tau^{\mathsf{CPA}}(z_2). \tag{10}$$

$\tilde{J}^{\alpha}$ in Eq. (7) is related to the current operator by $\tilde{J}^{\alpha} = D^{\alpha t} J^{\alpha} D^{\alpha}$, where D^{α} is the CPA impurity operator with respect to the component α and $D^{\alpha t}$ is the corresponding transposed operator (Faulkner and Stocks 1980).

The quantity ω in Eq. 7 contains the CPA single-site t-matrix t^{CPA} and the CPA scattering-path operator τ^{CPA}. Using an auxiliary quantity x^{α} defined as:

$$x^{\alpha}(z) = \left[1 - \Delta m^{\alpha}(z)\tau^{\mathsf{CPA}}(z)\right] \Delta m^{\alpha}(z), \tag{11}$$

with $\Delta m^{\alpha} = (t^{\mathsf{CPA}})^{-1} - (t^{\alpha})^{-1}$, $\omega(z_1, z_2)$ is given by:

$$\omega(z_1, z_2) = \sum_{\alpha} c^{\alpha} x^{\alpha}(z_1) x^{\alpha}(z_2). \tag{12}$$

Eq. 7 includes all contributions to the electrical conductivity. If one approximates the right hand side of Eq. 12 by the product of the average:

$$\left(\sum_{\alpha} c^{\alpha} x^{\alpha}(z_1)\right) \left(\sum_{\alpha} c^{\alpha} x^{\alpha}(z_2)\right), \tag{13}$$

$\omega = 0$, because the CPA condition implies that each term in round brackets in Eq. 13 vanishes. In Eq. 7 this approximation leads to a considerable simplification because the term marked "VC" then reduces to a unity matrix. This simplification corresponds to a suppression of vertex corrections to the electrical conductivity. One can assess the importance of these corrections by simply calculating the conductivity with and without this simplification.

Without vertex corrections the Kubo-Greenwood equation simplifies considerably:

$$\begin{aligned} \sigma_{\mu\mu}(\epsilon) &= -\frac{m_e^2}{\pi\hbar^3\Omega} \Bigg\{ \frac{1}{\Omega_{\mathrm{BZ}}} \int_{\mathrm{BZ}} d^3k \left[\sum_{\substack{\alpha\beta \\ z_1, z_2}} c^{\alpha} c^{\beta} s_{z_1, z_2} \, \tilde{J}^{\alpha\mu}(z_2, z_1)\tau(\vec{k}, z_1)\tilde{J}^{\beta\mu}(z_1, z_2)\tau(\vec{k}, z_2) \right] \\ &+ \sum_{\substack{\alpha\beta \\ z_1, z_2}} c^{\alpha} c^{\beta} s_{z_1, z_2} \, \tilde{J}^{\alpha\mu}(z_2, z_1) \, \tau^{\mathsf{CPA}}(z_1) \left(J^{\alpha\mu}(z_1, z_2) - \tilde{J}^{\beta\mu}(z_1, z_2) \right) \tau^{\mathsf{CPA}}(z_2) \Bigg\}. \end{aligned} \tag{14}$$

and now merely contains an integral over 3 scalar quantities instead an integral over the much larger matrix in Eq. 10.

An evaluation of Eqs. 7 or 14 is possible once the KKR–CPA equations have been solved and the scattering-path operator τ^{CPA} has been determined. What remains to be done is to calculate the current operators in the corresponding relativistic or non-relativistic representation and, for Eq. 7, to calculate the Brillouin zone average of a product of two inverse KKR–matrices $\tau(\vec{k}, z)$ in an efficient way.

3 Current operators

In this section explicit expressions for the non-relativistic and the relativistic current matrix elements and the relation between the current operators J^x, J^y and J^z are derived. Moreover, the non-relativistic operators are related to the relativistic ones.

3.1 Non-relativistic expression

In the framework of non-relativistic theory the current operator is given by

$$\vec{j} = \frac{e}{m_e}\vec{p} = -\frac{ie\hbar}{m_e}\vec{\nabla} \tag{15}$$

and the matrix elements needed for the evaluation of the Kubo-Greenwood equation are:

$$J^{\alpha\mu}_{LL'}(z_1, z_2) = -\frac{ie\hbar}{m_e}\int\limits_{\mathrm{WS}} d^3r Z^{\alpha *}_{L}(\vec{r}, z_1)\frac{\partial}{\partial r_\mu} Z^{\alpha}_{L'}(\vec{r}, z_2), \tag{16}$$

where the indices $L = (\ell, m_\ell)$ denote an angular momentum representation based on complex spherical harmonics:

$$Z^{\alpha}_{L}(\vec{r}, z) = R^{\alpha}_{\ell}(r, z) Y^{m_\ell}_{\ell}(\vartheta, \varphi). \tag{17}$$

The integral over the Wigner-Seitz cell can be replaced by an integral over the entire space by using a shape function for the Wigner-Seitz cell and by substituting

$$\hat{R}^{\alpha}_{\ell}(r) = R^{\alpha}_{\ell}(r)\Theta^{\mathrm{WS}}(\vec{r}\,), \quad \text{where} \quad \Theta^{\mathrm{WS}}(\vec{r}\,) = \begin{cases} 1 & \vec{r} \in \mathrm{WS} \\ 0 & \text{otherwise} \end{cases} \tag{18}$$

for R^{α}_{ℓ}. For a spherical domain (e.g. a muffin tin sphere of radius r_{MT} or a sphere corresponding to the Wigner-Seitz sphere with radius r_{WS}) $\Theta^{\mathrm{WS}}(\vec{r}\,) = \Theta(r_{\mathrm{MT}} - r)$ or $\Theta^{\mathrm{WS}}(\vec{r}\,) = \Theta(r_{\mathrm{WS}} - r)$, respectively. Using this expression and applying the gradient formula (Rose 1957) for spherical harmonics the derivative in Eq. 16 can be written as:

$$\begin{aligned}\frac{\partial}{\partial r_\mu}\left[\hat{R}^\alpha_{\ell'}(r)Y^{m_{\ell'}}_{\ell'}\right] &= \left[-\sqrt{\frac{\ell'+1}{2\ell'+1}}\left(\frac{\partial}{\partial r}\hat{R}^\alpha_{\ell'}(r)-\ell'\frac{\hat{R}^\alpha_{\ell'}(r)}{r}\right)\right.\\ &\sum_{k=-1}^{1}C(\ell'+1,1,\ell',m_{\ell'}-k,k,m_{\ell'})Y^{m_{\ell'}-k}_{\ell'+1}(\vec{\xi}_k)_\mu\\ &+\sqrt{\frac{\ell'}{2\ell'+1}}\left(\frac{\partial}{\partial r}\hat{R}^\alpha_{\ell'}(r)+(\ell'+1)\frac{\hat{R}^\alpha_{\ell'}(r)}{r}\right)\\ &\left.\sum_{k=-1}^{1}C(\ell'-1,1,\ell',m_{\ell'}-k,k,m_{\ell'})Y^{m_{\ell'}-k}_{\ell'-1}(\vec{\xi}_k)_\mu\right]. \end{aligned} \tag{19}$$

The vectors $\vec{\xi}$ are given by:

$$\vec{\xi}_1=-\frac{1}{\sqrt{2}}(1,i,0)\quad \vec{\xi}_0=(0,0,1)\quad \vec{\xi}_{-1}=\frac{1}{\sqrt{2}}(1,-i,0) \tag{20}$$

and C are the usual Clebsch-Gordan coefficients $C(l,s,j,m_l,m_s,m_j)$.
Inserting this expression into Eq. 16 and exploiting the orthogonality of the spherical harmonics $Y_l^{m_l}$ yields a closed expression for the current matrix elements corresponding to a spherical integration domain (e.g. a muffin tin sphere, MT):

$$\begin{aligned}J^{\alpha\mu,\mathrm{MT}}_{LL'} &= -\frac{i\hbar}{m_e}\\ &\left\{-\sqrt{\tfrac{\ell'+1}{2\ell'+1}}\left(\int_0^{r_{\mathrm{MT}}}r^2dr R^\alpha_\ell(r)\left[\frac{\partial}{\partial r}R^\alpha_{\ell'}(r)-\frac{\ell'}{r}R^\alpha_\ell(r)R^\alpha_{\ell'}(r)\right]-\frac{R^\alpha_\ell(r_{\mathrm{MT}})R^\alpha_{\ell'}(r_{\mathrm{MT}})r^2_{\mathrm{MT}}}{2}\right)\right.\\ &\times\sum_{k=-1}^{1}C(\ell'+1,1,\ell',m_{l'}-k,k,m_{l'})\delta_{\ell,\ell'+1}\delta_{m_l,m_l-k}(\vec{\xi}_k)_\mu+\\ &+\sqrt{\tfrac{\ell'}{2\ell'+1}}\left(\int_0^{r_{\mathrm{MT}}}r^2dr R^\alpha_\ell(r)\left[\frac{\partial}{\partial r}R^\alpha_{\ell'}(r)+\frac{\ell'+1}{r}R^\alpha_\ell(r)R^\alpha_{\ell'}(r)\right]-\frac{R^\alpha_\ell(r_{\mathrm{MT}})R^\alpha_{\ell'}(r_{\mathrm{MT}})r^2_{\mathrm{MT}}}{2}\right)\\ &\left.\times\sum_{k=-1}^{1}C(\ell'-1,1,\ell',m_{l'}-k,k,m_{l'})\delta_{\ell,\ell'-1}\delta_{m_l,m_{l'}-k}(\vec{\xi}_k)_\mu\right\}. \end{aligned} \tag{21}$$

The matrix structure of J^x and J^z is given in Tab. 1 and 2, respectively. Because the current matrices are not independent of each other, only one such matrix has to be calculated. The other components can then be obtained by exploiting the commutation relations $[L^z,J^x]=i\hbar J^y$ and $[L^x,J^y]=i\hbar J^z$:

$$J^y_{LL'} = -i(m_\ell - m_{\ell'})J^x_{LL'} \tag{22}$$

and

$$\begin{aligned} J^z_{LL'} \;=\; & \frac{1}{2i}\sum_{L''}\Big[\\ & \Big(\sqrt{\ell''(\ell''+1) - m_{\ell''}(m_{\ell''}+1)}\,\delta_{m_\ell,m_{\ell''}+1} + \sqrt{\ell''(\ell''+1) - m_{\ell''}(m_{\ell''}-1)}\,\delta_{m_\ell,m_{\ell''}-1}\Big)\delta_{\ell,\ell''}J^y_{L''L'} \\ & -\Big(\sqrt{\ell'(\ell'+1) - m_{\ell'}(m_{\ell'}+1)}\,\delta_{m_{\ell''},m_{\ell'}+1} + \sqrt{\ell'(\ell'+1) - m_{\ell'}(m_{\ell'}-1)}\,\delta_{m_{\ell''},m_{\ell'}-1}\Big)\delta_{\ell'',\ell'}J^y_{LL''}\Big] \end{aligned} \tag{23}$$

If the domain of integration in Eq. 16 is not a sphere, the integration in Eq. 21 can be carried out using a set of special directions. In this case the symmetry is lower and extra matrix elements occur in the current matrix. In Tabs. 1 and 2 these elements are marked by lower case letters for the case of cubic symmetry of the domain.

3.2 Relativistic expression

The relativistic current operator is defined in terms of the relativistic velocity operator:

$$\vec{j} = e\vec{v} = ec\vec{\alpha}, \tag{24}$$

where $\vec{\alpha}$ are the Dirac matrices (Rose 1961). The matrix elements needed for the evaluation of the Kubo-Greenwood equation are:

$$J^{\alpha\mu}_{\Lambda\Lambda'}(z_1,z_2) = ec\int\limits_{\rm WS} d^3r\; Z^{\dagger\alpha}_{\Lambda}(\vec{r},z_1)\;\alpha_\mu\; Z^{\alpha}_{\Lambda'}(\vec{r},z_2) \tag{25}$$

where $\Lambda = (\kappa, m_j)$ denotes a representation in terms of spin-angular functions (Rose 1961). In this representation the scattering solutions Z are of the form:

$$Z^\alpha_\Lambda(\vec{r},z) = \begin{pmatrix} g^\alpha_\kappa(r,z)\chi^{m_j}_\kappa \\ if^\alpha_\kappa(r,z)\chi^{m_j}_{-\kappa} \end{pmatrix} \tag{26}$$

and

$$Z^{\dagger\alpha}_\Lambda(\vec{r},z) = \left(g^\alpha_\kappa(r,z)\chi^{\dagger m_j}_\kappa,\; -if^\alpha_\kappa(r,z)\chi^{\dagger m_j}_{-\kappa}\right). \tag{27}$$

The Dirac matrices are defined in terms of the Pauli matrices:

$$\alpha_\mu = \begin{pmatrix} 0 & \sigma_\mu \\ \sigma_\mu & 0 \end{pmatrix}. \tag{28}$$

Because the matrices σ merely act on χ and not on the radial functions the current matrices can be written as:

$$J^{\alpha\mu}_{\Lambda\Lambda'} = eci \int\limits_{\mathrm{WS}} d^3r \left(g^\alpha_\kappa(r) f^\alpha_{\kappa'}(r) \chi^{\dagger m_j}_\kappa \sigma_\mu \chi^{m_{j'}}_{-\kappa'} - f^\alpha_\kappa(r) g^\alpha_{\kappa'}(r) \chi^{\dagger m_j}_{-\kappa} \sigma_\mu \chi^{m_{j'}}_{\kappa'} \right). \tag{29}$$

If the integration volume refers to spherical symmetry this result can be further simplified to

$$J^{\alpha\mu,\mathrm{MT}}_{\Lambda\Lambda'} = eci \left(R^\alpha_{\kappa,\kappa'} W^{\mu,m_j,m_{j'}}_{\kappa,-\kappa'} - R^\alpha_{\kappa',\kappa} W^{\mu,m_j,m_{j'}}_{-\kappa,\kappa'} \right), \tag{30}$$

where

$$R^\alpha_{\kappa\kappa'} = \int\limits_0^{r_{\mathrm{MT}}} r^2 dr \; g^\alpha_\kappa(r) f^\alpha_{\kappa'}(r) \tag{31}$$

and

$$W^{\mu,m_j,m_{j'}}_{\kappa\kappa'} = \int d\Omega \; \chi^{\dagger,m_j}_\kappa \sigma_\mu \chi^{m_{j'}}_{\kappa'}. \tag{32}$$

Because, as in the non-relativistic case, the current operators depend on each other, calculation of e.g. the x-component is sufficient:

$$W^{x,m_j m_{j'}}_{\kappa\kappa'} = \delta_{\ell,\ell'} \sum_{m_s} C(\ell, \frac{1}{2}, j, m_j - m_s, m_s, m_j) C(\ell', \frac{1}{2}, j', m_{j'} + m_s, -m_s, m_{j'}) \; \delta_{m_j, m_{j'}+2m_s}. \tag{33}$$

The structure of the current matrices J^x and J^z is shown in Tabs. 3 and 4, respectively. For integration volumes with lower than spherical symmetry extra matrix elements occur indicated by lower case letters in Tabs. 3 and 4 for cubic symmetry.

As in the case of the non-relativistic current matrix elements the various spatial components are related to each other. Using the commutation relations between J and L one obtains:

$$J^y_{\Lambda\Lambda'} = -i(m_j - m_{j'}) J^x_{\Lambda\Lambda'} \tag{34}$$

and

$$J^z_{\Lambda\Lambda'} = \frac{1}{2i} \quad \sum_{\Lambda''}\sum_{m_s}\Bigg[C(\ell,\frac{1}{2},j,m_\ell,m_s,m_j)C(\ell'',\frac{1}{2},j'',m''_\ell,m_s,m''_j)\times \tag{35}$$
$$\Big(\sqrt{\ell''(\ell''+1)-m''_\ell(m''_\ell+1)}\delta_{m_\ell,m''_\ell+1}+\sqrt{\ell''(\ell''+1)-m''_\ell(m''_\ell-1)}\delta_{m_\ell,m''_\ell-1}\Big)\delta_{\ell,\ell''}J^y_{\Lambda''\Lambda'}$$
$$-C(\ell'',\frac{1}{2},j'',m''_\ell,m_s,m''_j)C(\ell',\frac{1}{2},j',m'_\ell,m_s,m'_j)\times$$
$$\Big(\sqrt{\ell'(\ell'+1)-m'_\ell(m'_\ell+1)}\delta_{m''_\ell,m_{\ell'}+1}+\sqrt{\ell'(\ell'+1)-m'_\ell(m'_\ell-1)}\delta_{m''_\ell,m'_\ell-1}\Big)\delta_{\ell'',\ell'}J^y_{\Lambda\Lambda''}\Bigg]$$

3.3 Relation between non-relativistic and relativistic current operators

The relativistic current operator can be expanded yielding the non-relativistic expression as a leading term plus corrections in the order of $1/c^2$ (Wang and Callaway 1973) and higher ones:

$$\vec{j} = \frac{e}{m_e}\left[-i\hbar\vec{\nabla}+\frac{\hbar}{4m_ec^2}\vec{\sigma}\times\vec{\nabla}V(\vec{r})+\ldots\right] = \vec{j}^{(0)}+\vec{j}^{(1)}+\ldots, \tag{36}$$

where V ist the potential of the system and $\vec{\sigma}$ is the Dirac spin operator.

To allow for a direct comparison of non-relativistic ($\vec{j}^{(0)}$) and relativistic ($\vec{j}$) current operators, one has to calculate the nonrelativistic current operator in the relativistic representation. The evaluation is analogous to that of Eq. 21. The result for the matrix elements $J^{\alpha\mu,\mathrm{MT}}_{\Lambda\Lambda'}$ is similar to Eq. 21 except that it contains extra Clebsch-Gordan coefficients and two contributions corresponding to the g and the f component of the Dirac four-spinor. No mixed terms occur as they do in Eq. 31. The operators $-ie\hbar/m_e\vec{\nabla}$ and $ec\vec{\alpha}$ can then be directly compared.

The first correction term in Eq. 36 can also be calculated in a fairly simple way. Due to the cross product one has to calculate two terms of the form

$$\sigma_\mu\frac{\partial V(\vec{r})}{\partial r_\nu} \tag{37}$$

for each component of $\vec{\sigma}\times\vec{\nabla}V$. The expression $\partial V/\partial r_\nu$ can be transformed to spherical coordinates and expressed in terms of complex spherical harmonics:

$$\frac{\partial V(\vec{r})}{\partial r_\nu} = \frac{\partial V(\vec{r})}{\partial r}\times\begin{cases}\sin\vartheta\cos\varphi\\ \sin\vartheta\sin\varphi\\ \cos\vartheta\end{cases} = \frac{\partial V(\vec{r})}{\partial r}\times\begin{cases}\sqrt{\frac{2\pi}{3}}(Y_1^{-1}-Y_1^1), & \nu=x\\ i\sqrt{\frac{2\pi}{3}}(Y_1^{-1}+Y_1^1), & \nu=y\\ \sqrt{\frac{4\pi}{3}}Y_1^0, & \nu=z\end{cases} \tag{38}$$

Using the scattering solutions of Eqs. 26 and 27 one can then write:

$$\begin{aligned}
\int\limits_{\mathrm{MT}} d^3r Z^{\dagger\alpha}_{\Lambda}(\vec{r},z_1)\left[\sigma_\mu \frac{\partial V(\vec{r})}{\partial r_\nu}\right] Z^{\alpha}_{\Lambda'}(\vec{r},z_2) &= \sqrt{\frac{4\pi}{3}}\int\limits_0^{r_{\mathrm{MT}}} r^2 dr g_\kappa(r)^\alpha g^\alpha_{\kappa'}(r)\frac{\partial V(\vec{r})}{\partial r} \\
&\times \sum_{m_s,m_{s'}} C(\ell,\frac{1}{2},j,m_\ell,m_s,m_j)C(\ell',\frac{1}{2},j',m'_\ell,m'_s,m'_j) \\
&\times \sigma_{m_s,m'_s}\begin{cases} \frac{1}{2}(\mathcal{G}^{(1,-1)}_{L,L'}-\mathcal{G}^{(1,1)}_{L,L'}), & \nu=x \\ \frac{i}{2}(\mathcal{G}^{(1,-1)}_{L,L'}+\mathcal{G}^{(1,1)}_{L,L'}), & \nu=y \\ \mathcal{G}^{(1,0)}_{L,L'}, & \nu=z \end{cases} \\
&+ \text{corresponding f contribution} \qquad (39)
\end{aligned}$$

Here σ_{m_s,m'_s} denote the matrix elements of the ordinary 2×2 Pauli matrices. The triple products of spherical harmonics occuring in Eq. 39 have been represented by Gaunt coefficients $\mathcal{G}$ defined as:

$$\mathcal{G}^{L''}_{L,L'} = \int d\Omega \left(Y^{m_\ell}_\ell\right)^* Y^{m'_\ell}_{\ell'} Y^{m''_\ell}_{\ell''} \qquad (40)$$

There are six contributions which have to be calculated using Eq. 39 and put together to yield the first correction $\vec{j}^{(1)}$ to the non-relativistic current operator $\vec{j}^{(0)}$.

4 Brillouin zone average of two inverse KKR matrices

Solving the KKR–CPA equations requires an integration of the inverse KKR-matrix $\tau(\vec{k},z)$ over the Brillouin zone in order to obtain the CPA scattering-path operator τ^{CPA} (Eq. 8). In practice this means that each of the matrix elements $\tau_{QQ'}(\vec{k},z)$ has to be integrated separately. This task is simplified if one takes into account that many of these matrix elements vanish or are related to each other due to symmetry. Solving Eq. 10 means integration of each element $\tau_{QQ'}(\vec{k},z_1)\tau_{Q''Q'''}(\vec{k},z_2)$ over the Brillouin zone. For a relativistic representation and $\ell_{\max} = 3$, e.g., there are 32^4 such elements to integrate. Therefore, it is essential to know the matrix structure of χ^{CPA} in order to be able to compute χ^{CPA} efficiently. Moreover, in most cases an integration over the entire Brillouin zone is not necessary but can be reduced to the irreducible part (IBZ) by making use of the rotation group $\mathcal{P}$ corresponding to the underlying crystal structure. For cubic symmetry, e.g., there are 48 such point group symmetry operations and the Brillouin zone integrals can be reduced to integrals over one 1/48-th of the zone. The general expression is given by:

$$\tau^{\mathsf{CPA}}_{QQ'}(z) = \frac{1}{\Omega_{\mathrm{BZ}}}\int\limits_{IBZ} d^3k \sum_{R\in\mathcal{P}}\sum_{Q_1Q_2} D_{QQ_1}(R)\tau_{Q_1Q_2}(\vec{k},z)D^\dagger_{Q_2Q'}(R) \qquad (41)$$

$$\chi^{\mathsf{CPA}}_{QQ'Q''Q'''}(z_1,z_2) = \frac{1}{\Omega_{\mathrm{BZ}}}\int_{IBZ} d^3k \sum_{R\in\mathcal{P}} \sum_{\substack{Q_1Q_2\\Q_3Q_4}} D_{QQ_1}(R)\tau_{Q_1Q_2}(\vec{k},z)D^{\dagger}_{Q_2Q'}(R)D_{Q''Q_3}(R)\tau_{Q_3Q_4}(\vec{k},z)D^{\dagger}_{Q_4Q'''}(R) \quad (42)$$

where the matrices $D(R)$ contain blockwise the Clebsch-Gordan coefficients of the irreducible representation of $R \in \mathcal{P}$. $\mathcal{P}$ refers to the point group of order $|\mathcal{P}|$. Regrouping the matrix elements one obtains:

$$\tau^{\mathsf{CPA}}_{QQ'}(z) = \frac{1}{\Omega_{\mathrm{BZ}}}\int_{IBZ} d^3k \sum_{Q_1Q_2} S^{(Q_1Q_2)}_{QQ'}\tau_{Q_1Q_2}(\vec{k},z) \quad (43)$$

with

$$S^{(Q_1Q_2)}_{QQ'} = \sum_{R\in\mathcal{P}} D_{QQ_1}(R)D^{\dagger}_{Q_2Q'}(R) \quad (44)$$

and

$$\chi^{\mathsf{CPA}}_{QQ'Q''Q'''}(z_1,z_2) = \frac{1}{\Omega_{\mathrm{BZ}}}\int_{IBZ} d^3k \sum_{\substack{Q_1Q_2\\Q_3Q_4}} R^{(Q_1,Q_2,Q_3,Q_4)}_{QQ'Q''Q'''}\tau_{Q_1Q_2}(\vec{k},z_1)\tau_{Q_3Q_4}(\vec{k},z_2) \quad (45)$$

with

$$R^{(Q_1,Q_2,Q_3,Q_4)}_{QQ'Q''Q'''} = \sum_{R\in\mathcal{P}} D_{QQ_1}(R)D^{\dagger}_{Q_2Q'}(R)D_{Q''Q_3}(R)D^{\dagger}_{Q_4Q'''}(R) \quad (46)$$

Fortunately, many of the coefficients S and R vanish. If, e.g., for a given pair (QQ') all $S^{(QQ')}_{Q_1Q_2}$ vanish, the corresponding matrix element $\tau^{\mathsf{CPA}}_{QQ'}$ is zero. Identical elements of τ can be found in the following way: one chooses two elements $\tau_{QQ'}$ and $\tau_{PP'}$. Then one compares the two matrices $S^{(Q_1Q_2)}_{QQ'}$ and $S^{(P_1P_2)}_{PP'}$ element by element. If the matrices are identical the two elements of τ are identical. For χ the same can be done with the only difference that matrices with four indices have to be compared.

The matrix structure of τ^{CPA} and χ^{CPA} was analyzed in this way for cubic crystal symmetry. For τ^{CPA} one recovers the well known matrix structure (Staunton et al. 1980; Weinberger 1990). Tab. 5 shows, how many numerically different values the matrices τ^{CPA} and χ^{CPA} contain (not counting the zero value). As one can see, the number is comparatively small. In a calculation of χ^{CPA} one can therefore restrict the evaluation and integration of the integrand $\tau_{Q_1Q_2}(\vec{k},z_1)\tau_{Q_3Q_4}(\vec{k},z_2)$ to the set of indices identified this way. The indices have to be only calculated once and can be kept in tabulated form.

Note that the number of different elements for $\ell_{\max} = 2$ in the non-relativistic representation given in Tab. 5 (40) differs from a value (114) given by Swihart et al. (1986).

5 Complex energies

The evaluation of Eq. 6 requires the determination of operators for complex energies which lie above and below the real axis. In normal electronic structure calculations, however, only energies $\epsilon + i\eta$ with a positive imaginary part are usually encountered so that care has to be taken when energies $\epsilon - i\eta$ are involved as it is the case in conductivity calculations. For $\eta \to 0$ there are fairly simple relations between the various quantities $A(\epsilon + i\eta)$ and $A(\epsilon - i\eta)$ used in the calculation, where A is any of the operators of interest in the current context. These relations shall be derived now.

Because one is mostly dealing with energies which lie in the continuous spectrum of the alloy hamiltonian, one has to choose a path from $\epsilon + i\eta$ to $\epsilon - i\eta$ which avoids the discontinuous branch cut along the real axis (Economou 1983). A possible path describing an angle of 2π is shown in Fig. 1. One can write:

$$\epsilon - i\eta = \underbrace{e^{2\pi i}}_{1}(\epsilon + i\eta) \qquad \text{for} \quad \eta \to 0. \tag{47}$$

5.1 Wave vector

On the energy shell $k^2 = \epsilon$ (in atomic units which are used throughout this section). Denoting for a moment $k_z = \sqrt{z}, z = \epsilon \pm \eta$, on can write

$$k_{\epsilon - i\eta} = \sqrt{\epsilon - i\eta} = \sqrt{e^{2\pi i}}\sqrt{\epsilon + i\eta} = e^{\pi i}\sqrt{\epsilon + i\eta} = -\sqrt{\epsilon + i\eta} = -k_{\epsilon + i\eta}. \tag{48}$$

5.2 Phase shifts

The scattering behaviour of a spherically symmetrical scatterer can be charactersised by its phase shifts. These shifts can be written as (Weinberger 1990):

$$\cot \delta_\ell = \frac{\gamma_\ell n_\ell(kr) - k n'_\ell(kr)}{\gamma_\ell j_\ell(kr) - k j'_\ell(kr)}, \tag{49}$$

where $\gamma = R'/R$ is the logarithmic derivative at the sphere boundary. The Bessel- and Neumann functions and their derivatives satisfy the following parity relations (Abramowitz and Stegun 1964):

$$\begin{aligned} j_\ell(-kr) &= (-1)^\ell j_\ell(kr) \qquad & n_\ell(-kr) &= (-1)^{\ell+1} n_\ell(kr) \\ j'_\ell(-kr) &= (-1)^{\ell+1} j'_\ell(kr) & n'_\ell(-kr) &= (-1)^\ell n'_\ell(kr). \end{aligned} \tag{50}$$

This yields:

$$\cot\left[\delta_\ell(\epsilon+i\eta)\right] = -\cot\left[\delta_\ell(\epsilon-i\eta)\right]. \tag{51}$$

The same relation holds for the relativistic phase shifts.

5.3 t-matrix and scattering amplitude

The single-site t-matrix t and the scattering amplitude f can be expressed in terms of the phase shift:

$$t_{QQ'}(\epsilon+i\eta) = -\frac{1}{k}\underbrace{e^{i\delta_Q(\epsilon+i\eta)}\sin\left[\delta_Q(\epsilon+i\eta)\right]}_{f_Q}\delta_{QQ'}. \tag{52}$$

Using Eq. 48 one obtains:

$$\begin{aligned} f_Q(\epsilon-i\eta) &= -f_Q^*(\epsilon+i\eta) \\ t_{QQ'}(\epsilon-i\eta) &= t_{QQ'}^*(\epsilon+i\eta) \end{aligned} \tag{53}$$

5.4 Wave functions and current matrix elements

The solution of the wave equation in a constant potential can be written as (Weinberger 1990):

$$Z_\Lambda^{\text{free}}(\epsilon+i\eta,r) = \begin{cases} k\left(n_\ell(kr) - \cot\delta_\kappa j_\ell(kr)\right)\chi_\kappa^{m_j} \\ i\frac{\text{sgn}(\kappa)k^2}{c}\left(n_{\bar{\ell}}(kr) - \cot\delta_\kappa j_{\bar{\ell}}(kr)\right)\chi_{-\kappa}^{m_j} \end{cases}, \tag{54}$$

when the Dirac equation is used. Using Eqs. 48-51 one obtains:

$$Z_\Lambda^{\text{free}}(\epsilon-i\eta,r) = (-1)^\ell Z_\Lambda^{\text{free}}(\epsilon+i\eta,r). \tag{55}$$

As the wave functions in the muffin tin sphere are continuously matched to the free functions at the muffin tin sphere, Eq. 55 also applies to the wave function in the entire Wigner-Seitz cell. For the current matrix elements one then easily obtains the following relations:

$$\begin{aligned} J_{QQ'}^{\alpha\mu}(\epsilon-i\eta,\epsilon-i\eta) &= (-1)^{l+l'}J_{QQ'}^{\alpha\mu}(\epsilon+i\eta,\epsilon+i\eta) \\ J_{QQ'}^{\alpha\mu}(\epsilon-i\eta,\epsilon+i\eta) &= (-1)^{l}J_{QQ'}^{\alpha\mu}(\epsilon+i\eta,\epsilon+i\eta) \\ J_{QQ'}^{\alpha\mu}(\epsilon+i\eta,\epsilon-i\eta) &= (-1)^{l'}J_{QQ'}^{\alpha\mu}(\epsilon+i\eta,\epsilon+i\eta), \end{aligned} \tag{56}$$

5.5 k-space structure constants and scattering operators

The k-space structure constants for energies with negative imaginary part $z = \epsilon - i\eta$ can now be derived from the usual structure constants for $z = \epsilon + i\eta$ by substituting each $k = \sqrt{\epsilon}$ occurring in the corresponding expression for G^0 by $-k$. One can use an expression for G^0 given by Davis (1971), where a trivial diagonal part is separated off the actual structure constants B:

$$G^0_{QQ'}(\vec{k}, \epsilon + i\eta) = B_{QQ'}(\vec{k}, \epsilon + i\eta) + i\sqrt{\epsilon}\,\delta_{QQ'}, \tag{57}$$

An evaluation of these structure constants B yields:

$$G^0_{QQ'}(\vec{k}, \epsilon - i\eta) = (-1)^{l-l'} B_{QQ'}(\vec{k}, \epsilon + i\eta) - i\sqrt{\epsilon}\,\delta_{QQ'}. \tag{58}$$

For $\tau(\vec{k}, \epsilon)$ given by Eq. 9 a very similar expression can be derived:

$$\tau_{QQ'}(\vec{k}, \epsilon - i\eta) = (-1)^{l-l'} \left(\tau_{Q'Q}(\vec{k}, \epsilon + i\eta)\right)^*. \tag{59}$$

If one integrates $\tau(\vec{k}, \epsilon)$ over the Brillouin zone, all matrix elements with $\Delta\ell \neq 2n$ vanish and the resulting integrated matrix is symmetric thus yielding:

$$\tau^{\mathsf{CPA}}_{QQ'}(\epsilon - i\eta) = \tau^{\mathsf{CPA}}_{QQ'}(\epsilon + i\eta)^*. \tag{60}$$

6 Summary

The details of the application of the Kubo-Greenwood equation for the electrical conductivity to disordered alloys in the framework of the Korringa-Kohn-Rostoker version of the coherent potential approximation (KKR–CPA) are given. Both a non-relativistic and a relativistic version of the formalism has been worked out. Explicit expressions for the current matrix elements are given in both versions and for the first correction term to the non-relativistic current operator. The relations between operators at complex energies just above and below the real axis are derived. Moreover, it is shown how one can use symmetry considerations to facilitate the tedious calculation of the Brillouin zone average of two inverse KKR matrices needed for the evaluation of the Kubo-Greenwood equation.

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Tables

ℓ	s	p			d					f						
m_l	0	-1	0	1	-2	-1	0	1	2	-3	-2	-1	0	1	2	3
1		A		-A						a		b		-b		a
2	-A				B		C		c							
3						D		-D								
4	A				-c		-C		-B							
5		-B		c						E		F		d		e
6			-D								G		H		f	
7		-C		C						g		I		-I		-g
8			D								-f		-H		-G	
9		-c		B						-e		-d		-F		-E
10	-a				-E		-g		e							
11						-G		f								
12	-b				-F		-I		d							
13						-H		H								
14	b				-d		I		F							
15						-f		G								
16	-a				-e		g		E							

Table 1: Structure of the non-relativistic current matrix J^x for angular momenta up to $\ell = 3$. Capital letters: components corresponding to a spherical integration domain, lower case letters: additional components arising from a Wigner-Seitz cell with cubic symmetry. The matrix is hermitean and all components are purely imaginary. The selection rules are $\Delta\ell = \pm 1$, $\Delta m_\ell = \pm 1$ (spherical symmetry) and $\Delta\ell = \pm 1, 3 \ldots$, $\Delta m_\ell = \pm 1, 3 \ldots$ (cubic symmetry).

ℓ	s	p			d					f						
m_l	0	-1	0	1	-2	-1	0	1	2	-3	-2	-1	0	1	2	3
1			A										a			
2						B										
3	-A						C									
4								B								
5											D				b	
6		-B										E				c
7			-C										F			
8				-B						c				E		
9											b				D	
10								-c								
11					-D				-b							
12						-E										
13	-a						-F									
14								-E								
15					-b				-D							
16						-c										

Table 2: Structure of the non-relativistic current matrix J^z for angular momenta up to $\ell = 3$. Capital letters: components corresponding to a spherical integration domain, lower case letters: additional components arising from a Wigner-Seitz cell with cubic symmetry. The matrix is hermitean and all components are purely imaginary. The selection rules are $\Delta\ell = \pm 1$, $\Delta m_\ell = 0$ (spherical symmetry) and $\Delta\ell = \pm 1, 3 \ldots$, $\Delta m_\ell = 0, \pm 4 \ldots$ (cubic symmetry).

$\ell_j \rightarrow$	s1/2		p1/2		p3/2				d3/2				d5/2					
$m_j \rightarrow$	$+\frac{1}{2}$	$-\frac{1}{2}$	$+\frac{1}{2}$	$-\frac{1}{2}$	$+\frac{3}{2}$	$+\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{3}{2}$	$+\frac{3}{2}$	$+\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{3}{2}$	$+\frac{5}{2}$	$+\frac{3}{2}$	$+\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{3}{2}$	$-\frac{5}{2}$
1				A	B		C											
2			A			-C		-B										
3		-A							D		E			a		b		c
4	-A									-E		-D	c		b		a	
5	-B									F		d	G		H		e	
6		C							F		K			L		M		f
7	-C									K		F	-f		-M		-L	
8		-B							d		F			-e		-H		-G
9			-D			-F		-d										
10				E	-F		-K											
11			-E			-K		-F										
12				D	-d		-F											
13				-c	-G		f											
14			-a			-L		e										
15				-b	-H		M											
16			-b			-M		H										
17				-a	-e		L											
18			-c			-f		G										

Table 3: Structure of the relativistic current matrix elements J^x for angular momenta up to $\ell = 2$. Capital letters: components corresponding to a spherical domain, lower case letters: additional components arising from a Wigner-Seitz cell with cubic symmetry. The matrix is hermitean and all components are purely imaginary. The selection rules are $\Delta\ell = \pm 1$ and $\Delta m_j = \pm 1$ for spherical symmetry, $\Delta\ell = \pm 1, 3 \ldots$ and $\Delta m_j = \pm 1, 3 \ldots$ for cubic symmetry).

ℓ_j	s1/2		p1/2		p3/2				d3/2				d5/2					
m_j	$+\frac{1}{2}$	$-\frac{1}{2}$	$+\frac{1}{2}$	$-\frac{1}{2}$	$+\frac{3}{2}$	$+\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{3}{2}$	$+\frac{3}{2}$	$+\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{3}{2}$	$+\frac{5}{2}$	$+\frac{3}{2}$	$+\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{3}{2}$	$-\frac{5}{2}$
1			A			B												
2				-A			B											
3	-A									C					a			
4		A									C					-a		
5									D					E				b
6	-B									F					G			
7		-B									-F					G		
8												-D	b				E	
9					-D													
10			-C			-F												
11				-C			F											
12								D										
13								-b										
14					-E													
15			-a			-G												
16				a			-G											
17								-E										
18					-b													

Table 4: Structure of the relativistic current matrix elements J^z for angular momenta up to $\ell = 2$. Capital letters: components corresponding to a spherical domain, lower case letters: additional components arising from a Wigner-Seitz cell with cubic symmetry. The matrix is hermitean and all components are purely imaginary. The selection rules are $\Delta\ell = \pm 1$ and $\Delta m_j = 0$ for spherical symmetry, $\Delta\ell = \pm 1, 3\ldots$ and $\Delta m_j = 0, \pm 4\ldots$ for cubic symmetry).

	non-relativistic		relativistic					
	(ℓ, m_ℓ) representation		γ representation		Λ representation		(ℓ, m_ℓ, m_s) representation	
$\ell_{\max}$	τ^{CPA}	χ^{CPA}	τ^{CPA}	χ^{CPA}	τ^{CPA}	χ^{CPA}	τ^{CPA}	χ^{CPA}
1	2	2	3	24	3	24	5	28
2	4	40	7	648	11	686	14	702
3	13	512	17	5334	not det.			

Table 5: Number of numerically different elements of the CPA-scattering-path operator τ and the Brillouin-zone averaged product χ^{CPA}. For χ only elements with $\Delta\ell = \pm 1$ have been taken into account. Elements with different signs are considered identical. Non-relativistic representation: (ℓ,m_ℓ)-representation (real spherical harmonics), relativistic representations: Λ-, γ-, and (ℓ,m$_\ell$,m$_s$)-representation (see Staunton, Gyorffy and Weinberger 1980 for definitions of the relativistic representations).

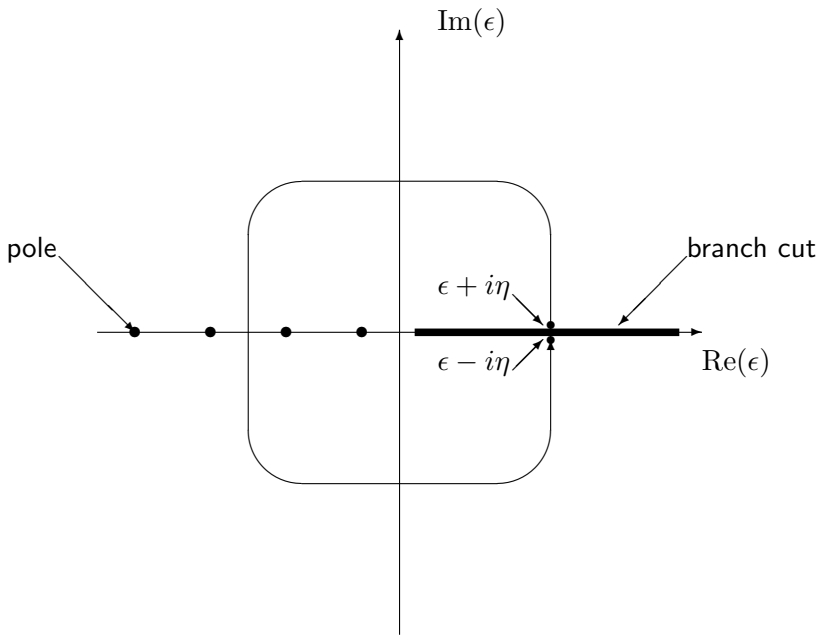

Figure 1: Schematical representation of the spectrum of $G(\epsilon)$ showing a path from $\epsilon + i\eta$ to $\epsilon - i\eta$ (for $\eta \to 0$).