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‘Band structure’ and electrical conductivity of disordered layered systems

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Abstract. Employing the Kubo–Greenwood formula, the electrical conductivity of disordered layered systems is formulated in terms of the (screened) Korringa–Kohn–Rostoker method and the coherent potential approximation. It is shown that the elements of the electrical conductivity tensor can be described in terms of ‘layer-diagonal’ and ‘layer-off-diagonal’ contributions. In order to discuss effects of the underlying electronic structure on the electrical conductivity, but also to point out particular contributions to it, Bloch spectral functions are formulated. A spin-polarized (relativistic) application of the present theory to non-collinear disordered magnetic multilayers allows one to discuss giant magnetoresistance (GMR) on an *ab initio* level in quite a general context.

1. Introduction

The giant magnetoresistance of magnetic multilayers is interesting both for the physics needed to explain its origins and because of its applicability to emerging computer technologies [1]. Although there is a consensus that this effect comes from the magnetic field changing the spin dependent scattering of the conduction electrons, there are several ‘open questions’ both experimental and theoretical. Among the outstanding ones is that of whether it is the dependence of the electronic ‘band structure’ of a multilayer system on the orientation of the magnetization in the magnetic layers or the intrinsic spin-dependence of the single site scattering potentials that is the dominant cause for the magnetoresistance observed in these structures. An *ab initio* calculation of the electrical conductivity for magnetic multilayer systems implies as a first stage a self-consistent determination of the electronic structure of the ferromagnetic and antiferromagnetic configurations of a given system, including a total energy calculation to ascertain which configuration is the ground state. To determine the electrical conductivity or resistivity, however, one has to introduce scattering into a perfect system such as impurities in the bulk part of a layered system, geometrical roughness and chemical interdiffusion at the interfaces, grain boundaries and magnetic domain walls. We will focus our attention on the scattering arising from interdiffused interfaces, since the spin-dependent scattering in the magnetic multilayers which display giant magnetoresistance (GMR) is concentrated especially at interfaces. The algorithm

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for calculating the conductivity of random homogeneous alloys, namely the KKR CPA (Korringa–Kohn–Rostoker coherent potential approximation) approach, has been shown to be quite successful [2]. First attempts to extend this kind of approach to layered systems by employing the layer KKR CPA were made by Butler *et al* [3–6]. The results up to now have already led to interesting physical insights, although they seem to be not quite compatible with the experimental size of the MR. The present paper is based on the general applicability of the so-called screened KKR CPA (SKKR CPA) method for layered systems [7], which makes use of a 'surface Green's function' approach and which has already been applied successfully in the context of non-relativistic [7], relativistic [8] and spin-polarized relativistic multiple scattering [9]. In section 2 the inhomogeneous CPA condition for layered systems is discussed in terms of 'traditional' multiple-scattering theory, followed by section 3 on Bloch spectral functions, which ultimately are the only tool to describe 'band structure effects' in disordered layered systems. Finally, in close relationship to these Bloch spectral functions, the electrical conductivity for interdiffused interfaces is derived in section 4 . It should be noted that the derived quantities are in principle also valid for any non-collinear magnetic structure of magnetic multilayers if the spin-polarized relativistic version of the SKKR CPA is applied. The differences between our paper and those of Butler *et al* [4–6] are that (i) we give details of the derivation of equation (55) from equation (36); in particular we distinguish between the different averaging procedures for site-diagonal and site-off diagonal contributions; and (ii) we show the similitude between the site-diagonal scattering path operators entering Bloch spectral functions and those entering the conductivity. In particular we point out the 'sum rule' equation (26) that these functions must satisfy.

2. The CPA condition for layered systems

Consider a situation as shown in figure 1, namely a multilayer system with interdiffused layers; that is, a system, which at best has only two-dimensional translational symmetry. A theoretically similar situation would for example occur at the surface of a binary alloy with an inhomogeneous concentration profile in the surface region. Suppose that such a layered system corresponds to a parent infinite (three-dimensionally periodic) system consisting of a simple lattice with only one atom per unit cell, then any lattice site $\boldsymbol{R}_{pi}$ can be written as

$$\boldsymbol{R}_{pi} = \boldsymbol{C}_p + \boldsymbol{R}_i \qquad \boldsymbol{R}_i \in L_2 \tag{1}$$

where $\boldsymbol{C}_p$ is the 'spanning vector' of a particular layer p and the two-dimensional (real) lattice is denoted by $L_2 = \{\boldsymbol{R}_i\}$ with the corresponding set of indices $I(L_2)$. For a given intermediate region of n layers, a multilayer, that is sandwiched by a left and a right semi-inifinite system (see also figure 1), the coherent scattering path operator $\tau_c(z)$ is given by the following surface Brillouin zone (SBZ) integral [7],

$$\tau_c^{pi,qj}(z) = \Omega_{SBZ}^{-1} \int \exp\left[-\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{R}_i - \boldsymbol{R}_j)\right] \widehat{\tau}_c^{pq}(\boldsymbol{k}, z)\mathrm{d}^2k \tag{2}$$

which implies two-dimensional translational invariance of the coherent medium for all layers of the intermediate region (multilayer), namely that in each layer p for the coherent single-site t-matrices $t_c(z)$ the following translational invariance applies:

$$t_c^{pi}(z) = t_c^{p}(z) \qquad \forall i \in I(L_2). \tag{3}$$

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 $\widehat{\tau}_c^{pq}(\boldsymbol{k}, z)$ in (2) for layered structures are provided by different variants of multiple scattering theory [7, 10–12]. In the following supermatrices labelled by layers only and denoted by a 'hat' symbol shall be used:

$$\widehat{t}_c(z) = \begin{pmatrix} \widehat{t}_c^{11}(z) & 0 & \cdots & & 0 \\ & \ddots & & & \\ 0 & \cdots & \widehat{t}_c^{pp}(z) & \cdots & 0 \\ & & & \ddots & \\ 0 & & \cdots & 0 & \widehat{t}_c^{nn}(z) \end{pmatrix} \tag{4}$$

with $\widehat{t}_c^{pp}(z) \equiv t_c^p(z)$ and

$$\widehat{\tau}_c(z) = \begin{pmatrix} & \vdots & & \vdots & \\ \cdots & \widehat{\tau}_c^{pp}(z) & \cdots & \widehat{\tau}_c^{pq}(z) & \cdots \\ & \vdots & & \vdots & \\ \cdots & \widehat{\tau}_c^{qp}(z) & \cdots & \widehat{\tau}_c^{qq}(z) & \cdots \\ & \vdots & & \vdots & \end{pmatrix} \qquad p, q = 1, \ldots, n. \tag{5}$$

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

$$\widehat{\tau}_c^{pq}(z) = \tau_c^{pi,qi}(z) = \tau_c^{p0,q0}(z) = \Omega_{SBZ}^{-1} \int \widehat{\tau}_c^{pq}(\boldsymbol{k}, z)\, \mathrm{d}^2k \tag{6}$$

refers to the unit cells at the origin of L_2 in layers p and q. Equation (6) also explains the notation used in (1). Suppose now that the concentration for constituents A and B in layer p is denoted by c_p^α $(p = 1, \ldots, n)$, and one specifies the occupation in the unit cell at the origin of L_2 of a particular layer p in terms of the following matrix $\widehat{m}_{p\alpha}(z)$:

$$\widehat{m}_{p\alpha}(z) = \begin{pmatrix} 0 & & \cdots & & \\ & \ddots & & & \\ 0 & \cdots & m_\alpha^p(z) & \cdots & 0 \\ & & & \ddots & \\ & & \cdots & & 0 \end{pmatrix} \tag{7}$$

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

where $t_\alpha^p(z)$ is the single-site t-matrix for constituent α in layer p. The corresponding layer-diagonal element of the so-called impurity matrix is then given by

$$\widehat{D}_\alpha^{pp}(z) \equiv D_\alpha^{p0,p0}(z) = \left[1 - m_\alpha^p(z)\tau_c^{p0,p0}(z)\right]^{-1} = \left\{1 - \left[\widehat{m}_{p\alpha}(z)\widehat{\tau}_c(z)\right]^{pp}\right\}^{-1} \tag{8}$$

and specifies a single impurity of type α in the translational invariant 'host' formed by layer p. The coherent scattering path operator for the intermediate region (multilayer) $\widehat{\tau}_c(z)$, is therefore obtained from the following inhomogeneous CPA condition (see also [15]):

$$\widehat{\tau}_c^{pp}(z) = \sum_{\alpha=A,B} c_p^\alpha \left\langle \widehat{\tau}^{pp}(z) \right\rangle_{p,\alpha} \quad \left\langle \widehat{\tau}^{pp}(z) \right\rangle_{p,\alpha} = \widehat{\tau}_\alpha^{pp}(z) = \widehat{D}_\alpha^{pp}(z)\widehat{\tau}_c^{pp}(z) \quad p = 1, \ldots, n \tag{9}$$

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

$$\left\langle \widehat{\tau}^{pp}(z) \right\rangle_{p,\alpha} \equiv \left\langle \tau^{p0,p0}(z) \right\rangle_{p0,\alpha} = \left\langle \tau^{pi,pi}(z) \right\rangle_{pi,\alpha} \qquad \forall i \in I(L_2) \qquad p = 1, \ldots, n. \tag{10}$$

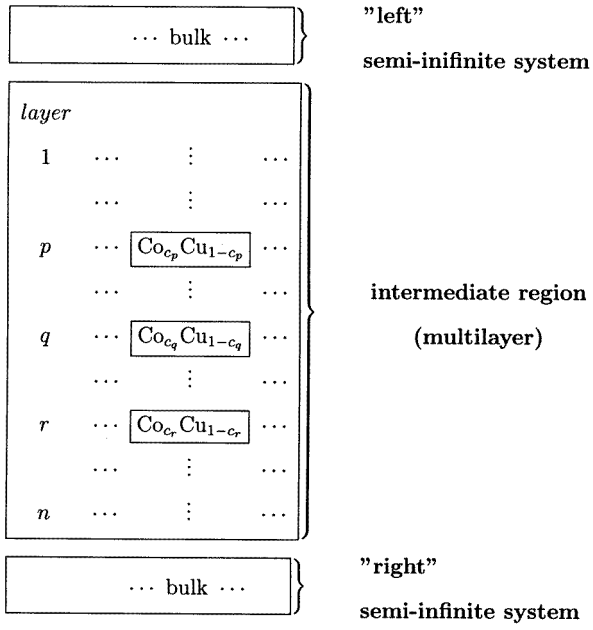

Figure 1. A typical multilayer system containing n interdiffused Co/Cu layers. Note that in each layer p in the intermediate region $0 \leqslant c_p \leqslant 1$.

Similarly, by specifying the occupation on two different sites [13, 14] the following restricted averages are obtained:

$$\left\langle \tau^{pi,qj}(z) \right\rangle_{pi\alpha,qj\beta} = \widehat{D}^{pp}_{\alpha}(z)\tau_c^{pi,qj}(z)\widehat{D}^{qq}_{\beta}(z)^t \qquad \forall i, j \in I(L_2) \tag{11}$$

for $p \neq q$ and

$$\left\langle \tau^{pi,pj}(z) \right\rangle_{pi\alpha,pj\beta} = \widehat{D}^{pp}_{\alpha}(z)\tau_c^{pi,pj}(z)\widehat{D}^{pp}_{\beta}(z)^t \qquad \forall (i \neq j) \in I(L_2) \tag{12}$$

for $p = q$, where $\left\langle \tau_c^{pi,qj}(z) \right\rangle_{pi\alpha,qj\beta}$ has the meaning that site (sub-cell) pi is occupied by species α and site (sub-cell) qj by species β and the symbol t indicates a transposed matrix.

3. Bloch spectral functions

3.1. Definitions

For real energies the imaginary part of the configurationally averaged Green function can be written as

$$\begin{aligned} \mathrm{Im}\left\langle G(\boldsymbol{r}, \boldsymbol{r}'; \epsilon) \right\rangle = {} & \delta_{pq}\,\delta_{ij}\mathrm{Im}\sum_{\alpha=A,B} c_{\alpha}^{p} \sum_{\Lambda\Lambda'} Z_{\Lambda}^{p\alpha}(\boldsymbol{r}_{pi}; \epsilon) \left\langle \tau_{c,\Lambda\Lambda'}^{pi,pi}(\epsilon) \right\rangle_{pi,\alpha} Z_{\Lambda'}^{p\alpha}(\boldsymbol{r}_{pi}; \epsilon)^{\dagger} \\ & + (1 - \delta_{pq}\,\delta_{ij})\mathrm{Im}\sum_{\alpha,\beta=A,B} c_{\alpha}^{p} c_{\beta}^{q} \sum_{\Lambda\Lambda'} Z_{\Lambda}^{p\alpha}(\boldsymbol{r}_{pi}; \epsilon) \left\langle \tau_{c,\Lambda\Lambda'}^{pi,qj}(\epsilon) \right\rangle_{pi\alpha,qj\beta} Z_{\Lambda'}^{q\beta}(\boldsymbol{r}_{qj}; \epsilon)^{\dagger} \end{aligned} \tag{13}$$

where $\boldsymbol{r} = \boldsymbol{r}_{pi} + \boldsymbol{R}_{pi}$ and $\boldsymbol{r}' = \boldsymbol{r}_{qj} + \boldsymbol{R}_{qj}$, the $Z_{\Lambda}^{p\alpha}(\boldsymbol{r}_{pi}, \epsilon)$ are the scattering solutions [13, 14] corresponding to component α with respect to site $i \in I(L_2)$ in layer p and Λ refers to

the appropriate set of angular momentum indices such as $\Lambda = (\ell m)$ in a non-relativistic approach. Obviously, (13) can be re-formulated in terms of a SBZ integral:

$$\mathrm{Im}\left\langle G(\boldsymbol{r}_{pi}+\boldsymbol{R}_{pi}, \boldsymbol{r}_{qj}+\boldsymbol{R}_{qj}; \epsilon)\right\rangle = \Omega_{SBZ}^{-1}\int \exp\left[-\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{R}_i - \boldsymbol{R}_j)\right] \times \left\langle G^{pq}(\boldsymbol{r}_{pi}, \boldsymbol{r}_{qj}; \boldsymbol{k}, \epsilon)\right\rangle \mathrm{d}^2k \tag{14}$$

where the $\boldsymbol{k}$th projection of the Green function, $\left\langle G^{pq}(\boldsymbol{r}_{pi}, \boldsymbol{r}_{qj}; \boldsymbol{k}, \epsilon)\right\rangle$ is given by

$$\left\langle G^{pq}(\boldsymbol{r}_{pi}, \boldsymbol{r}_{qj}; \boldsymbol{k}, \epsilon)\right\rangle = \sum_{j\in I(L_2)} \exp\left(-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}_j\right)\left\langle G(\boldsymbol{r}_p+\boldsymbol{C}_p, \boldsymbol{r}_q+\boldsymbol{C}_q+\boldsymbol{R}_j; \epsilon)\right\rangle. \tag{15}$$

Bloch spectral functions $A_B(\boldsymbol{k}, \epsilon)$ are then defined as [13, 14]

$$A_B(\boldsymbol{k}, \epsilon) = -\pi^{-1}\mathrm{Im}\mathrm{Tr}\left\langle G(\boldsymbol{k}, \epsilon)\right\rangle = \sum_{p=1}^{n} A^p(\boldsymbol{k}, \epsilon) \tag{16}$$

$$A^p(\boldsymbol{k}, \epsilon) = -\pi^{-1}\mathrm{Im}\int_{\Omega_{p0}} \left\langle G^{pp}(\boldsymbol{r}_{p0}, \boldsymbol{r}_{p0}; \boldsymbol{k}, \epsilon)\right\rangle d^3r_{p0} \tag{17}$$

where Tr denotes a trace over a supermatrix in layer indices and the tensorial space of spin and configuration, and Ω_{p0} refers to the volume of the $p0$th unit cell.

3.2. Evaluation of Bloch spectral functions

For matters of proper averaging it is useful to split up $A^p(\boldsymbol{k}, \epsilon)$ into two terms,

$$A^p(\boldsymbol{k}, \epsilon) = A_0^p(\epsilon) + A_1^p(\boldsymbol{k}, \epsilon). \tag{18}$$

The first type of contribution (the diagonal contribution), namely $A_0^p(\epsilon)$, refers to the averaging at the origin of L_2 of layer p:

$$A_0^p(\epsilon) = -\pi^{-1}\sum_{\alpha=A,B} c_p^\alpha \,\mathrm{Im}\,\mathrm{tr}\left[\left\langle\tau^{p0,p0}(\epsilon)\right\rangle_{p0,\alpha} F_p^{\alpha\alpha}(\epsilon)\right] = -\pi^{-1}\sum_{\alpha=A,B} c_p^\alpha \,\mathrm{Im}\,\mathrm{tr} \times \left[\widehat{D}_\alpha^{pp}(\epsilon)\widehat{\tau}_c^{pp}(\epsilon)F_p^{\alpha\alpha}(\epsilon)\right] \tag{19}$$

where the following matrices $F_p^{\alpha\beta}(\epsilon)$ have been introduced:

$$F_p^{\alpha\beta}(\epsilon) \equiv \left\{F_{p,\Lambda\Lambda'}^{\alpha\beta}(\epsilon)\right\} \qquad \alpha = A, B \qquad F_{p,\Lambda\Lambda'}^{\alpha\beta}(\epsilon) = \int_{\Omega_{p0}} Z_\Lambda^{p\alpha}(\boldsymbol{r}_{p0}, \epsilon)^\dagger Z_{\Lambda'}^{p\beta}(\boldsymbol{r}_{p0}, \epsilon)\,\mathrm{d}^3r_{p0} \tag{20}$$

and tr indicates a trace of a matrix in angular momentum space. The second type of contribution (the off-diagonal contribution) deals with different pairs (unit cells) in one and the same layer:

$$A_1^p(\boldsymbol{k}, \epsilon) = -\pi^{-1}\sum_{\alpha,\beta=A,B} c_p^\alpha c_p^\beta \mathrm{Im}\,\mathrm{tr}\left(\sum_{(j\neq 0)\in I(L_2)} \exp\left(-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}_j\right)\left\langle\tau^{p0,pj}(\epsilon)\right\rangle_{p0\alpha,pj\beta} F_p^{\alpha\beta}(\epsilon)\right) \tag{21}$$

which by using (12) can be transformed into

$$A_1^p(\boldsymbol{k}, \epsilon) = -\pi^{-1}\sum_{\alpha,\beta=A,B} c_p^\alpha c_p^\beta \times \mathrm{Im}\,\mathrm{tr}\left[\widehat{D}_\alpha^{pp}(\epsilon)\left(\sum_{(j\neq 0)\in I(L_2)} \exp\left(-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}_j\right)\tau_c^{p0,pj}(\epsilon)\right)\widehat{D}_\beta^{pp}(\epsilon)^t F_p^{\alpha\beta}(\epsilon)\right]. \tag{22}$$

If the restricted sum in the last equation is extended to $\forall j \in I(L_2)$ and the corresponding $j = 0$ contribution is subtracted, equation (22) can be expressed in terms of the $\boldsymbol{k}$th projection of the layer-diagonal scattering path operator, $\widehat{\tau}_c^{pp}(\boldsymbol{k}, \epsilon)$:

$$A_1^p(\boldsymbol{k}, \epsilon) = -\pi^{-1} \sum_{\alpha,\beta=A,B} c_p^\alpha c_p^\beta \left\{ \mathrm{Im\,tr} \left[\widehat{D}_\alpha^{pp}(\epsilon) \widehat{\tau}_c^{pp}(\boldsymbol{k}, \epsilon) \widehat{D}_\beta^{pp}(\epsilon)^t F_p^{\alpha\beta}(\epsilon) \right] \right.$$
$$\left. - \mathrm{Im\,tr} \left[\widehat{D}_\alpha^{pp}(\epsilon) \widehat{\tau}_c^{pp}(\epsilon) \widehat{D}_\beta^{pp}(\epsilon)^t F_p^{\alpha\beta}(\epsilon) \right] \right\}. \tag{23}$$

It should be noted that, in comparison with the bulk case (simple lattice, one atom per unit cell), in which Bloch spectral functions are expressed in terms of *site-diagonal* scattering path operators [13, 14], for a layered system *layer-diagonal* scattering path operators occur. Layer-resolved Bloch spectral functions describe the electronic structure in a chosen layer. It is well known that, for ordered layers (systems), they consist of a set of Dirac δ-functions at the energetic positions of corresponding $\boldsymbol{k}$-resolved energy eigenvalues. For disordered layers (systems) more or less broad peaks have to be expected that vary with respect to energy ϵ and $\boldsymbol{k}$.

For bulk systems Bloch spectral functions are an important tool to discuss and understand Fermi surfaces and physical properties related to the topology of these surfaces. By calculating Bloch spectral functions along rays originating from the centre of the Brillouin zone, one can construct the Fermi surface by identifying the positions of the maxima of the Bloch spectral functions with the position of the various sheets of the Fermi surface in a given direction. The width of these maxima is a measure for the mean free path of the quasi-particles.

The Kubo–Greenwood equation offers a rigorous approach to the calculation of electrical resistivities. However, the result of such calculations merely consists of a single value for isotropical bulk systems and of a small number of layer-resolved conductivities for layered systems. Therefore, one would like to get more information in order to be able to interpret the results and to find schemes to explain them. Such information is offered by the use of Bloch spectral functions. Especially for highly anisotropic systems such as magnetic multilayers, the mean free paths as functions of $\boldsymbol{k}$ are expected to show a wealth of structure and will be a key for an interpretation of the Kubo–Greenwood conductivity results.

3.3. The layer-resolved density of states

Suppose that one would integrate the pth Bloch spectral function over the SBZ. It is fairly easy to see that the $\boldsymbol{k}$-independent diagonal contribution defined in (19) is a sum over concentration-weighted, component- and layer-projected densities of states $n_\alpha^p(\epsilon)$ [7]:

$$A_0^p(\epsilon) = \sum_{\alpha=A,B} c_p^\alpha n_\alpha^p(\epsilon) \tag{24}$$

$$n_\alpha^p(\epsilon) = -\pi^{-1} \mathrm{Im\,tr} \left[\widehat{D}_\alpha^{pp}(\epsilon) \widehat{\tau}_c^{pp}(\epsilon) F_p^{\alpha\alpha}(\epsilon) \right] \tag{25}$$

whereas the off-diagonal contribution cancels exactly

$$\Omega_{SBZ}^{-1} \int A_1^p(\boldsymbol{k}, \epsilon) \mathrm{d}^2 k = -\pi^{-1} \sum_{\alpha,\beta=A,B} c_p^\alpha c_p^\beta \left\{ \mathrm{Im\,tr} \left\{ \widehat{D}_\alpha^{pp}(\epsilon) \left[\Omega_{SBZ}^{-1} \int \widehat{\tau}_c^{pp}(\boldsymbol{k}, \epsilon) \mathrm{d}^2 k \right] \right.\right.$$
$$\left.\left. \times \widehat{D}_\beta^{pp}(\epsilon)^t F_p^{\alpha\beta}(\epsilon) \right\} - \mathrm{Im\,tr} \left[\widehat{D}_\alpha^{pp}(\epsilon) \widehat{\tau}_c^{pp}(\epsilon) \widehat{D}_\beta^{pp}(\epsilon)^t F_p^{\alpha\beta}(\epsilon) \right] \right\} = 0. \tag{26}$$

It can be seen that the 'correction term' in (22) and (23) is indeed important, since otherwise condition (26) is not fulfilled.

4. Conductivity for layered systems

4.1. General expressions

Suppose that the electrical conductivity of a disordered system, namely $\sigma_{\mu\nu}$, is calculated using the Kubo–Greenwood formula [2, 14, 16, 17]

$$\sigma_{\mu\nu} = \frac{\pi\bar{h}}{N_0\Omega_{at}}\left\langle \sum_{m,n} J^{\mu}_{mn} J^{\nu}_{nm}\delta(\epsilon_F - \epsilon_m)\delta(\epsilon_F - \epsilon_n)\right\rangle. \tag{27}$$

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

$$J^{\nu} = \left\{J^{\nu}_{nm}\right\} \qquad J^{\nu}_{nm} = \langle n \mid J_{\nu} \mid m\rangle \tag{28}$$

$|\, m\rangle$ 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. Equation (27) can be re-formulated in terms of the imaginary part of the (one-particle) Green function

$$\sigma_{\mu\nu} = \frac{\bar{h}}{\pi N_0\Omega_{at}}\mathrm{Tr}\,\left\langle J_{\mu} ImG^{+}(\epsilon_F) J_{\nu} ImG^{+}(\epsilon_F)\right\rangle. \tag{29}$$

or by using 'up-' and 'down-' side limits, this equation can be re-written [17] as

$$\sigma_{\mu\nu} = \tfrac{1}{4}\left[\widetilde{\sigma}_{\mu\nu}(\epsilon^{+}, \epsilon^{+}) + \widetilde{\sigma}_{\mu\nu}(\epsilon^{-}, \epsilon^{-}) - \widetilde{\sigma}_{\mu\nu}(\epsilon^{+}, \epsilon^{-}) - \widetilde{\sigma}_{\mu\nu}(\epsilon^{-}, \epsilon^{+})\right] \tag{30}$$

where

$$\begin{aligned} &\epsilon^{+} = \epsilon_F + \mathrm{i}\delta \qquad \epsilon^{-} = \epsilon_F - \mathrm{i}\delta \qquad \delta \to 0 \\ &\widetilde{\sigma}_{\mu\nu}(\epsilon_1, \epsilon_2) = -\frac{\bar{h}}{\pi N_0\Omega_{at}}\mathrm{tr}\,\left\langle J_{\mu} G(\epsilon_1) J_{\nu} G(\epsilon_2)\right\rangle \qquad \epsilon_i = \epsilon^{\pm} \qquad i = 1, 2. \end{aligned} \tag{31}$$

As in the bulk case [17, 14] a typical contribution to the conductivity can be expressed in terms of real-space scattering path operators

$$\begin{aligned} \widetilde{\sigma}_{\mu\nu}(\epsilon_1, \epsilon_2) = \frac{C}{N_0}\sum_{p=1}^{n}\Bigg[\sum_{i\in I(L_2)}\sum_{q=1}^{n}\Bigg(\sum_{j\in I(L_2)}\mathrm{tr}\Big\langle J^{pi}_{\mu}(\epsilon_2, \epsilon_1)\tau^{pi,qj} \\ \times (\epsilon_1) J^{qj}_{\nu}(\epsilon_1, \epsilon_2)\tau^{qj,pi}(\epsilon_2)\Big\rangle\Bigg)\Bigg] \end{aligned} \tag{32}$$

where $C = -4m^2/(\bar{h}^3\pi\Omega_{at})$ 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 (the number of atoms in one layer). Let $J^{p\alpha}_{\mu}(\epsilon_1, \epsilon_2)$ denote the angular momentum representation of the μth 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 $\boldsymbol{J} = [e\bar{h}/(\mathrm{i}m)]\boldsymbol{\nabla}$, the elements of $J^{p\alpha}_{\mu}(\epsilon_1, \epsilon_2)$ are given by

$$J^{p\alpha}_{\mu,\Lambda\Lambda'}(\epsilon_1, \epsilon_2) = \frac{e}{m}\frac{\bar{h}}{i}\int_{\mathrm{WS}} Z^{p\alpha}_{\Lambda}(\boldsymbol{r}_{p0}, \epsilon_1)^{\dagger}\frac{\partial}{\partial r_{p0,\mu}} Z^{p\alpha}_{\Lambda'}(\boldsymbol{r}_{p0}, \epsilon_2)\mathrm{d}^3 r_{p0} \tag{33}$$

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

$$J^{p\alpha}_{\mu,\Lambda\Lambda'}(\epsilon_1, \epsilon_2) = ec\int_{\mathrm{WS}} Z^{p\alpha}_{\Lambda}(\boldsymbol{r}_{p0}, \epsilon_1)^{\dagger}\alpha_{\mu} Z^{p\alpha}_{\Lambda'}(\boldsymbol{r}_{p0}, \epsilon_2)\mathrm{d}^3 r_{p0}. \tag{34}$$

In equations (33) and (34) the functions $Z_{\Lambda}^{p\alpha}(\boldsymbol{r}_{p0}, z)$ are again scattering solutions [14] and WS denotes the volume of the Wigner–Seitz sphere. It should be noted that

$$J_{\mu}^{p\alpha}(\epsilon_1, \epsilon_2) = J_{\mu}^{p0,\alpha}(\epsilon_1, \epsilon_2) = J_{\mu}^{pi,\alpha}(\epsilon_1, \epsilon_2) \qquad \forall i \in I(L_2). \tag{35}$$

From the brackets in (32), one easily can see that for each layer p the first sum over L_2 yields N times the same contribution, provided that two-dimensional invariance applies in all layers under consideration. Assuming this kind of symmetry (see section 2), a typical contribution $\widetilde{\sigma}_{\mu\nu}(\epsilon_1, \epsilon_2)$ to the conductivity is therefore given by

$$\widetilde{\sigma}_{\mu\nu}(\epsilon_1, \epsilon_2) = \frac{C}{n} \sum_{p=1}^{n} \sum_{q=1}^{n} \left(\sum_{j \in I(L_2)} \mathrm{tr} \left\langle J_{\mu}^{p0}(\epsilon_2, \epsilon_1) \tau^{p0,qj}(\epsilon_1) J_{\nu}^{qj}(\epsilon_1, \epsilon_2) \tau^{qj,p0}(\epsilon_2) \right\rangle \right) \tag{36}$$

where $p0$ specifies the origin of L_2 for the pth layer. Just as in the bulk case [17, 14] this kind of contribution can be split up into a (site-) diagonal and a (site-) off-diagonal part, namely

$$\widetilde{\sigma}_{\mu\nu}(\epsilon_1, \epsilon_2) = \widetilde{\sigma}_{\mu\nu}^{0}(\epsilon_1, \epsilon_2) + \widetilde{\sigma}_{\mu\nu}^{1}(\epsilon_1, \epsilon_2). \tag{37}$$

4.2. The site-diagonal conductivity

By employing the CPA condition in (9) and omitting vertex corrections, for the diagonal part ($p0 = qj$) one simply gets in terms of the definitions given in (6) and (35)

$$\begin{aligned} \widetilde{\sigma}_{\mu\nu}^{0}(\epsilon_1, \epsilon_2) &= \frac{C}{n} \sum_{p=1}^{n} \sum_{\alpha=A,B} c_p^{\alpha} \mathrm{tr} \left[J_{\mu}^{p\alpha}(\epsilon_2, \epsilon_1) \left\langle \widehat{\tau}^{pp}(\epsilon_1) \right\rangle_{p\alpha} J_{\nu}^{p\alpha}(\epsilon_1, \epsilon_2) \left\langle \widehat{\tau}^{pp}(\epsilon_2) \right\rangle_{p\alpha} \right] \\ &= \frac{C}{n} \sum_{p=1}^{n} \sum_{\alpha=A,B} c_p^{\alpha} \mathrm{tr} \left[J_{\mu}^{p\alpha}(\epsilon_2, \epsilon_1) \widehat{D}_{\alpha}^{pp}(\epsilon_1) \widehat{\tau}_c^{pp}(\epsilon_1) J_{\nu}^{p\alpha}(\epsilon_1, \epsilon_2) \widehat{D}_{\alpha}^{pp}(\epsilon_2) \widehat{\tau}_c^{pp}(\epsilon_2) \right] \\ &= \frac{C}{n} \sum_{p=1}^{n} \sum_{\alpha=A,B} c_p^{\alpha} \mathrm{tr} \left[\widetilde{J}_{\mu}^{p\alpha}(\epsilon_2, \epsilon_1) \widehat{\tau}_c^{pp}(\epsilon_1) J_{\nu}^{p\alpha}(\epsilon_1, \epsilon_2) \widehat{\tau}_c^{pp}(\epsilon_2) \right] \end{aligned} \tag{38}$$

where

$$\widetilde{J}_{\mu}^{p\alpha}(\epsilon_2, \epsilon_1) = \widehat{D}_{\alpha}^{pp}(\epsilon_2)^{t} J_{\mu}^{p\alpha}(\epsilon_2, \epsilon_1) \widehat{D}_{\alpha}^{pp}(\epsilon_1). \tag{39}$$

4.3. The site-off-diagonal conductivity

According to (11) and (12) the off-diagonal part can be partitioned into two terms:

$$\widetilde{\sigma}_{\mu\nu}^{1}(\epsilon_1, \epsilon_2) = \widetilde{\sigma}_{\mu\nu}^{2}(\epsilon_1, \epsilon_2) + \widetilde{\sigma}_{\mu\nu}^{3}(\epsilon_1, \epsilon_2) \tag{40}$$

where

$$\begin{aligned} \widetilde{\sigma}_{\mu\nu}^{2}(\epsilon_1, \epsilon_2) = \frac{C}{n} \sum_{p=1}^{n} \sum_{q=1}^{n} (1 - \delta_{pq}) \Bigg(\sum_{j \in I(L_2)} \mathrm{tr} \Big\langle & J_{\mu}^{p0}(\epsilon_2, \epsilon_1) \tau^{p0,qj}(\epsilon_1) \\ & \times J_{\nu}^{qj}(\epsilon_1, \epsilon_2) \tau^{qj,p0}(\epsilon_2) \Big\rangle \Bigg) \end{aligned} \tag{41}$$

$$\widetilde{\sigma}_{\mu\nu}^{3}(\epsilon_1, \epsilon_2) = \frac{C}{n} \sum_{p=1}^{n} \sum_{q=1}^{n} \delta_{pq} \left(\sum_{(j \neq 0) \in I(L_2)} \mathrm{tr} \left\langle J_{\mu}^{p0}(\epsilon_2, \epsilon_1) \tau^{p0,qj}(\epsilon_1) J_{\nu}^{qj}(\epsilon_1, \epsilon_2) \tau^{qj,p0}(\epsilon_2) \right\rangle \right). \tag{42}$$

As one can see, $\widetilde{\sigma}^2_{\mu\nu}(\epsilon_1,\epsilon_2)$ arises from pairs of sites located in *different* layers, whereas $\widetilde{\sigma}^3_{\mu\nu}(\epsilon_1,\epsilon_2)$ corresponds to pairs of sites in *one and the same* layer (excluding the site-diagonal pair already being accounted for in $\widetilde{\sigma}^0_{\mu\nu}(\epsilon_1,\epsilon_2)$). In general the averaging of $\widetilde{\sigma}^2_{\mu\nu}(\epsilon_1,\epsilon_2)$ is given by

$$\widetilde{\sigma}^2_{\mu\nu}(\epsilon_1,\epsilon_2)=\frac{C}{n}\Bigg(\sum_{p=1}^{n}\sum_{q=1}^{n}(1-\delta_{pq})\sum_{j\in I(L_2)}\sum_{\alpha,\beta=A,B}c_p^{\alpha}c_p^{\beta}\mathrm{tr}\Big[J_{\mu}^{p\alpha}(\epsilon_2,\epsilon_1)\Big\langle\tau^{p0,qj}(\epsilon_1)J_{\nu}^{qj}\times(\epsilon_1,\epsilon_2)\tau^{qj,p0}(\epsilon_2)\Big\rangle_{p0\alpha,qj\beta}\Bigg). \tag{43}$$

By employing the CPA condition and omitting vertex corrections, $\widetilde{\sigma}^2_{\mu\nu}(\epsilon_1,\epsilon_2)$ is found to reduce to

$$\widetilde{\sigma}^2_{\mu\nu}(\epsilon_1,\epsilon_2)=\frac{C}{n}\Bigg(\sum_{p=1}^{n}\sum_{q=1}^{n}(1-\delta_{pq})\sum_{j\in I(L_2)}\sum_{\alpha,\beta=A,B}c_p^{\alpha}c_q^{\beta}\mathrm{tr}\Big[J_{\mu}^{p\alpha}(\epsilon_2,\epsilon_1)\Big\langle\tau^{p0,qj}(\epsilon_1)\Big\rangle_{p0a,qj\beta}\times J_{\nu}^{q\beta}(\epsilon_1,\epsilon_2)\left\langle\tau^{qj,p0}(\epsilon_2)\right\rangle_{p0\alpha,qj\beta}\Big]\Bigg) \tag{44}$$

or, by using (11), to

$$\widetilde{\sigma}^2_{\mu\nu}(\epsilon_1,\epsilon_2)=\frac{C}{n}\Bigg(\sum_{p=1}^{n}\sum_{q=1}^{n}(1-\delta_{pq})\sum_{j\in I(L_2)}\sum_{\alpha,\beta=A,B}c_p^{\alpha}c_q^{\beta}\mathrm{tr}\Big[\widetilde{J}_{\mu}^{p\alpha}(\epsilon_2,\epsilon_1)\tau_c^{p0,qj}(\epsilon_1)\times\widetilde{J}_{\nu}^{q\beta}(\epsilon_1,\epsilon_2)\tau_c^{qj,p0}(\epsilon_2)\Big]\Bigg). \tag{45}$$

Since the site-off-diagonal scattering path operators $\tau_c^{p0,qj}(z)$ are defined according to (2) as

$$\tau_c^{p0,qj}(z)=\Omega_{SBZ}^{-1}\int \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}_j}\widehat{\tau}^{pq}(\boldsymbol{k},z)\mathrm{d}^2k \tag{46}$$

in a manner similar to that in the bulk case the orthogonality for irreducible representations of the two-dimensional translation group can be used:

$$\sum_{j\in I(L_2)}\tau_c^{p0,qj}(\epsilon_1)\tau_c^{qj,p0}(\epsilon_2)=\Omega_{SBZ}^{-1}\int\widehat{\tau}^{pq}(\boldsymbol{k},\epsilon_1)\widehat{\tau}^{qp}(\boldsymbol{k},\epsilon_2)\mathrm{d}^2k. \tag{47}$$

For $\widetilde{\sigma}^2_{\mu\nu}(\epsilon_1,\epsilon_2)$ one therefore gets the following expression

$$\widetilde{\sigma}^2_{\mu\nu}(\epsilon_1,\epsilon_2)=\frac{C}{n}\Bigg(\sum_{p=1}^{n}\sum_{q=1}^{n}(1-\delta_{pq})\,\Omega_{SBZ}^{-1}\sum_{\alpha,\beta=A,B}c_p^{\alpha}c_q^{\beta}\mathrm{tr}\int\Big[\widetilde{J}_{\mu}^{p\alpha}(\epsilon_2,\epsilon_1)\widehat{\tau}_c^{pq}(\boldsymbol{k},\epsilon_1)\times\widetilde{J}_{\nu}^{q\beta}(\epsilon_1,\epsilon_2)\widehat{\tau}_c^{qp}(\boldsymbol{k},\epsilon_2)\mathrm{d}^2k\Big]\Bigg). \tag{48}$$

The last term in (40) to be evaluated is $\widetilde{\sigma}^3_{\mu\nu}(\epsilon_1,\epsilon_2)$, which corresponds to the case that two sites are located in one and the same layer, namely

$$\widetilde{\sigma}^3_{\mu\nu}(\epsilon_1,\epsilon_2)=\frac{C}{n}\sum_{p=1}^{n}\Bigg(\sum_{(j\neq0)\in I(L_2)}\mathrm{tr}\left\langle J_{\mu}^{p0}(\epsilon_2,\epsilon_1)\tau^{p0,pj}(\epsilon_1)J_{\nu}^{pj}(\epsilon_1,\epsilon_2)\tau^{p0,pj}(\epsilon_2)\right\rangle\Bigg). \tag{49}$$

From the above discussion of $\widetilde{\sigma}^2_{\mu\nu}(\epsilon_1,\epsilon_2)$ it is easy to see that $\widetilde{\sigma}^3_{\mu\nu}(\epsilon_1,\epsilon_2)$ is given by

$$\widetilde{\sigma}^3_{\mu\nu}(\epsilon_1,\epsilon_2) = \frac{C}{n}\Bigg(\sum_{p=1}^{n}\Omega^{-1}_{SBZ}\sum_{\alpha,\beta=A,B} c_p^\alpha c_p^\beta \mathrm{tr}\int \widetilde{J}^{p\alpha}_\mu(\epsilon_2,\epsilon_1)\widehat{\tau}^{pp}_c(\boldsymbol{k},\epsilon_1)\widetilde{J}^{p\beta}_\nu(\epsilon_1,\epsilon_2)\widehat{\tau}^{pp}_c \times(\boldsymbol{k},\epsilon_2)\mathrm{d}^2k\Bigg) + \widetilde{\sigma}^{3,corr}_{\mu\nu}(\epsilon_1,\epsilon_2) \tag{50}$$

where $\widetilde{\sigma}^{3,corr}_{\mu\nu}(\epsilon_1,\epsilon_2)$ arises from the same kind of procedure that has been employed for the Bloch spectral functions, namely from extending the sum to $\forall j \in I(L_2)$ and subtracting a corresponding correction term of the form

$$\begin{aligned}\widetilde{\sigma}^{3,corr}_{\mu\nu}(\epsilon_1,\epsilon_2) &= -\frac{C}{n}\sum_{p=1}^{n}\sum_{\alpha,\beta=A,B} c_p^\alpha c_p^\beta \mathrm{tr}\Big[J^{p\alpha}_\mu(\epsilon_2,\epsilon_1)\widehat{D}^{pp}_\alpha(\epsilon_1)\widehat{\tau}^{pp}_c(\epsilon_1)\widehat{D}^{pp}_\beta(\epsilon_1)^t \\ &\quad\times J^{p\beta}_\nu(\epsilon_1,\epsilon_2)\widehat{D}^{pp}_\beta(\epsilon_2)\widehat{\tau}^{pp}_c(\epsilon_2)\widehat{D}^{pp}_\alpha(\epsilon_2)^t\Big] \\ &= -\frac{C}{n}\sum_{p=1}^{n}\sum_{\alpha,\beta=A,B} c_p^\alpha c_p^\beta \mathrm{tr}\big[\widetilde{J}^{p\alpha}_\mu(\epsilon_2,\epsilon_1)\widehat{\tau}^{pp}_c(\epsilon_1)\widetilde{J}^{p\beta}_\nu(\epsilon_1,\epsilon_2)\widehat{\tau}^{pp}_c(\epsilon_2)\big].\end{aligned} \tag{51}$$

4.4. The total conductivity for layered systems

Combining now all terms, a typical contribution $\widetilde{\sigma}_{\mu\nu}(\epsilon_1,\epsilon_2)$ to the conductivity is given by

$$\begin{aligned}\widetilde{\sigma}_{\mu\nu}(\epsilon_1,\epsilon_2) = \frac{C}{n}\sum_{p=1}^{n}\Bigg(&\sum_{\alpha=A,B} c_p^\alpha \mathrm{tr}\big[\widetilde{J}^{p\alpha}_\mu(\epsilon_2,\epsilon_1)\widehat{\tau}^{pp}_c(\epsilon_1)J^{p\alpha}_\nu(\epsilon_1,\epsilon_2)\widehat{\tau}^{pp}_c(\epsilon_2)\big] \\ &- \sum_{\alpha,\beta=A,B} c_p^\alpha c_p^\beta \mathrm{tr}\big[\widetilde{J}^{p\alpha}_\mu(\epsilon_2,\epsilon_1)\widehat{\tau}^{pp}_c(\epsilon_1)\widetilde{J}^{p\beta}_\nu(\epsilon_1,\epsilon_2)\widehat{\tau}^{pp}_c(\epsilon_2)\big] \\ &+\Omega^{-1}_{SBZ}\sum_{q=1}^{n}\sum_{\alpha,\beta=A,B} c_p^\alpha c_q^\beta \mathrm{tr}\int\Big[\widetilde{J}^{p\alpha}_\mu(\epsilon_2,\epsilon_1)\widehat{\tau}^{pq}_c(\boldsymbol{k},\epsilon_1)\widetilde{J}^{q\beta}_\nu(\epsilon_1,\epsilon_2)\widehat{\tau}^{qp}_c \\ &\times(\boldsymbol{k},\epsilon_2)\,\mathrm{d}^2k\Big]\Bigg).\end{aligned} \tag{52}$$

Comparing the last equation with the corresponding bulk result [17], one easily can see that in both cases one has the same 'formal structure', however, for layered systems a summation over layers occurs for the diagonal term and a double sum over layers for the off-diagonal term. Therefore, defining layer-diagonal terms as

$$\begin{aligned}\widetilde{\sigma}^{pp}_{\mu\nu}(\epsilon_1,\epsilon_2) = \frac{C}{n}\sum_{\alpha=A,B} c_p^\alpha\Bigg(&\mathrm{tr}\big[\widetilde{J}^{p\alpha}_\mu(\epsilon_2,\epsilon_1)\widehat{\tau}^{pp}_c(\epsilon_1)J^{p\alpha}_\nu(\epsilon_1,\epsilon_2)\widehat{\tau}^{pp}_c(\epsilon_2)\big] \\ &- \sum_{\beta=A,B} c_p^\beta \mathrm{tr}\Big[\widetilde{J}^{p\alpha}_\mu(\epsilon_2,\epsilon_1)\widehat{\tau}^{pp}_c(\epsilon_1)\widetilde{J}^{p\beta}_\nu(\epsilon_1,\epsilon_2)\widehat{\tau}^{pp}_c(\epsilon_2)\Big]\Bigg)\end{aligned} \tag{53}$$

and layer-off-diagonal terms as

$$\begin{aligned}\widetilde{\sigma}^{pq}_{\mu\nu}(\epsilon_1,\epsilon_2) = \frac{C}{n}\Omega_{SBZ})\sum_{\alpha,\beta=A,B} c_p^\alpha c_q^\beta \mathrm{tr}\Big[\int \widetilde{J}^{p\alpha}_\mu(\epsilon_2,\epsilon_1)\widehat{\tau}^{pq}_c(\boldsymbol{k},\epsilon_1)\widetilde{J}^{q\beta}_\nu(\epsilon_1,\epsilon_2)\widehat{\tau}^{qp}_c \\ \times(\boldsymbol{k},\epsilon_2)\mathrm{d}^2k\Big]\end{aligned} \tag{54}$$

$\widetilde{\sigma}_{\mu\nu}(\epsilon_1, \epsilon_2)$ can be written as

$$\widetilde{\sigma}_{\mu\nu}(\epsilon_1, \epsilon_2) = \sum_{p=1}^{n} \left(\widetilde{\sigma}_{\mu\nu}^{pp}(\epsilon_1, \epsilon_2) + \sum_{q=1}^{n} \widetilde{\sigma}_{\mu\nu}^{pq}(\epsilon_1, \epsilon_2) \right). \tag{55}$$

It should be noted that, as pointed out in section 2, all contributions are now defined in terms of the supermatrices $\widehat{\tau}_c(\epsilon_i)$ and $\widehat{\tau}_c(\boldsymbol{k}, \epsilon_i)$, $\epsilon_i = \epsilon^{\pm}$. It also should be recalled from the discussion of the Bloch spectral functions that $\widetilde{\sigma}_{\mu\nu}^{3,corr}(\epsilon_1, \epsilon_2)$, which is the second term in (52), plays an important role. Quite clearly (55) allows one to discuss the electrical conductivity of layered systems in terms of *intra-layer* and *inter-layer* contributions.

5. Discussion

It should be recalled that the screened KKR CPA method for multilayer systems (see in particular [7]) is based on the use of surface Green's functions, that is, the 'left' and the 'right' semi-infinite systems are 'glued' onto the intermediate region (multilayer) via surface Green's functions. A semi-infinite 'bulk' region can be either vacuum or a solid such as a pure metal, a substitutional alloy or an insulator (or semi-conductor). The present approach is therefore very flexible with respect to the actual experimental set-up. If, for example, multilayers are grown on an insulating substrate, this can also be taken into account very well in the same realistic manner as can statistically disordered alloys representing 'bulk' regions.

Vertex corrections do not affect the form of equation (55), but their inclusion does change the expressions in equations (53) and (54). They are omitted in our presentation for two reasons: (i) their inclusion complicates the expressions and obfuscates the meaning of the terms entering the conductivity, and (ii) to calculate the conductivity for currents in the plane of the layers (CIP) there are no vertex corrections to the layer conductivities (σ^{pq}) coming from the layered structure of the scattering; there are of course the corrections that enter from momentum-dependent scattering. However, this appears in homogeneous systems and we are interested in focusing on the new features involved in layered structures [19]. For currents perpendicular to the layers (CPP) the layered conductivity in this direction does have contributions from vertex corrections coming from the layered nature of the scattering. However, as we have shown, see for example [18], one can find the measured CPP conductivity by using the expressions (53) and (54) which omit these corrections. This is done by enforcing current conservation at a later step in the calculation. Butler *et al* have used this kind of recipe to calculate the CPP conductivity by using the layered conductivities that omit the vertex corrections (private communication). A detailed discussion of the effect of vertex corrections for bulk alloys is given in [20], in which it is shown that in fact errors due to truncation of angular momentum expansions are much bigger than those caused by neglecting vertex corrections! Quite clearly, just as in the case of the conceptually much easier bulk alloys, all approximations made, such as for the occurring angular momentum expansions, vertex corrections and relativistic corrections [20], will have to be checked in due course together with the $\boldsymbol{k}$-convergence of the SBZ integrals involved.

6. Summary

The above theory of the electrical conductivity of disordered layered systems, in particular its spin-polarized relativistic version, is applicable to any non-collinear magnetic configuration of a diffused (disordered) system of magnetic multilayers. Therefore it allows one to

discuss giant magnetoresistance (GMR) on an *ab initio* level in quite a general context. Section 3 not only provided a very valid argument for the importance of the 'correction term' in the layer-diagonal contributions to the conductivity but also showed that actual calculations of Bloch spectral functions at the Fermi energy for a particular magnetic configuration can provide considerable insight into the very details of the GMR. Since, furthermore, the optical conductivity tensor can be formulated in a similar manner and since magnetically coated surfaces are just another manifestation of layered systems, also *ab initio* calculations of magneto-optical properties for realistic systems are within reach. A necessary precondition for all such calculations, however, is that one evaluate $\widehat{\tau}_c(\epsilon_i)$ for a given profile of interdiffusion and for at least two magnetic configurations (for example 'ferromagnetic' and 'antiferromagnetic') self-consistently within the framework of density functional theory. This can be achieved rather efficiently using the screened KKR method for layered systems, which also serves as a computational tool in the evaluation of the surface Brillouin zone intergals needed to evaluate the electrical conductivity. Computer codes for these kinds of SBZ integrals are presently under investigation.

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