9 SCIENTIFIC HIGHLIGHT

Electrical conductivity of multilayer 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. In particular consequences with respect to bulk-like approaches and bulk-like concepts are pointed out. The present investigations are part of an intensive study of transport phenomena such as the Giant Magnetoresistance (GMR) and the Tunneling Magnetoresistance (TMR) in magnetic multilayers systems.

Introduction

A description of transport phenomena in multilayer systems requires conceptually new approaches that reflect the fact that such systems exhibit at best two-dimensional symmetry. However, in applying a new type of description, it is also mandatory to review typical bulk-like descriptions based on the use of three-dimensional translational symmetry, and to be able to recover results well-known from bulk studies. It is the aim of this contribution to show exactly these relations, but also to proof that the present numerical procedures are well-suited for theoretical studies of more complicated transport properties in multilayer systems such as the Giant Magnetoresistance or the Tunneling Magnetoresistance.

Theoretical description

General expressions

Suppose the electrical conductivity of a disordered system, namely $\sigma_{\mu\mu}$, is calculated using the Kubo-Greenwood formula (see [1], [2], [3], [4])

$$\sigma_{\mu\mu} = \frac{\pi\hbar}{N_0\Omega_{at}} \left\langle \sum_{m,n} J^{\mu}_{mn} J^{\mu}_{nm} \delta(\epsilon_F - \epsilon_m)\delta(\epsilon_F - \epsilon_n) \right\rangle \quad . \tag{1}$$

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

$$J^{\mu} = \{J^{\mu}_{nm}\} \quad ; \quad J^{\mu}_{nm} = \langle n \mid J_{\mu} \mid m \rangle \quad , \tag{2}$$

$\mid m\rangle$ 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. (1) can be reformulated in terms of the imaginary part of the (one-particle) Green's function

$$\sigma_{\mu\mu} = \frac{\hbar}{\pi N_0 \Omega_{at}} \mathrm{Tr} \ \langle J_{\mu} \mathrm{Im} G^{+}(\epsilon_F) J_{\mu} \mathrm{Im} G^{+}(\epsilon_F) \rangle \quad . \tag{3}$$

or by using "up-" and "down-" side limits, this equation can be rewritten [2] as

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

where

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

and

$$\widetilde{\sigma}_{\mu\mu}(\epsilon_1, \epsilon_2) = -\frac{\hbar}{\pi N_0 \Omega_{at}} \mathrm{tr} \ \langle J_{\mu} G(\epsilon_1) J_{\mu} G(\epsilon_2) \rangle \quad ; \quad \epsilon_i = \epsilon^{\pm} \quad ; \quad i = 1, 2 \quad . \tag{5}$$

The multiple scattering description

As in the bulk case [2], [3] for a layered system a typical contribution to the conductivity can be expressed [5] in terms of real space scattering path operators,

$$\begin{aligned} \widetilde{\sigma}_{\mu\mu}(\epsilon_1, \epsilon_2) \quad = \quad & (C/N_0) \sum_{p=1}^{n} \sum_{i \in I(L_2)} \sum_{q=1}^{n} \\ & \left\{ \sum_{j \in I(L_2)} \mathrm{tr} \left\langle J^{pi}_{\mu}(\epsilon_2, \epsilon_1) \tau^{pi,qj}(\epsilon_1) J^{qj}_{\mu}(\epsilon_1, \epsilon_2) \tau^{qj,pi}(\epsilon_2) \right\rangle \right\} \quad , \end{aligned} \tag{6}$$

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). In here and in the following the set of indices corresponding to the two-dimensional lattice L_2 is denoted by $I(L_2)$. Let $J^{p\alpha}_{\mu}(\epsilon_1, \epsilon_2)$ 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

$$J^{p\alpha}_{\mu,\Lambda\Lambda'}(\epsilon_1,\epsilon_2) = \frac{e}{m}\frac{\hbar}{i}\int\limits_{WS} Z^{p\alpha}_{\Lambda}(\mathbf{r}_{p0},\epsilon_1)^\dagger \frac{\partial}{\partial r_{p0,\mu}} Z^{p\alpha}_{\Lambda'}(\mathbf{r}_{p0},\epsilon_2) d^3r_{p0} \quad , \tag{7}$$

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

$$J^{p\alpha}_{\mu,\Lambda\Lambda'}(\epsilon_1,\epsilon_2) = ec\int\limits_{WS} Z^{p\alpha}_{\Lambda}(\mathbf{r}_{p0},\epsilon_1)^\dagger \alpha_\mu Z^{p\alpha}_{\Lambda'}(\mathbf{r}_{p0},\epsilon_2) d^3r_{p0} \quad . \tag{8}$$

In Eqs. (7), (8) the functions $Z^{p\alpha}_{\Lambda}(\mathbf{r}_{p0},z)$ are scattering solutions [3] and WS denotes the volume of the Wigner-Seitz sphere. It should be noted that

$$J^{p\alpha}_{\mu}(\epsilon_1,\epsilon_2) = J^{p0,\alpha}_{\mu}(\epsilon_1,\epsilon_2) = J^{pi,\alpha}_{\mu}(\epsilon_1,\epsilon_2) \quad , \quad \forall i \in I(L_2) \quad . \tag{9}$$

¿From the brackets in Eq. (6), one easily can see that for each layer p the first sum over L_2 yields N times the same contribution, provided two-dimensional invariance applies in all layers under consideration. Assuming this kind of symmetry (see Sec. II), a typical contribution $\widetilde{\sigma}_{\mu\mu}(\epsilon_1,\epsilon_2)$ to the conductivity is therefore given by

$$\begin{aligned}\widetilde{\sigma}_{\mu\mu}(\epsilon_1,\epsilon_2) &= (C/n)\sum_{p=1}^{n}\sum_{q=1}^{n} \\ &\left\{\sum_{j\in I(L_2)} \mathrm{tr}\left\langle J^{p0}_{\mu}(\epsilon_2,\epsilon_1)\tau^{p0,qj}(\epsilon_1)J^{qj}_{\mu}(\epsilon_1,\epsilon_2)\tau^{qj,p0}(\epsilon_2)\right\rangle\right\} \quad ,\end{aligned} \tag{10}$$

where $p0$ specifies the origin of L_2 for the p-th layer. Just as in the bulk case [2], [3] this kind of contribution can be split up into a (site-) diagonal and a (site-) off-diagonal part,

$$\widetilde{\sigma}_{\mu\mu}(\epsilon_1,\epsilon_2) = \widetilde{\sigma}^0_{\mu\mu}(\epsilon_1,\epsilon_2) + \widetilde{\sigma}^1_{\mu\mu}(\epsilon_1,\epsilon_2) \quad . \tag{11}$$

Site-diagonal conductivity

By employing the CPA condition discussed in full detail in Ref. [5] and omitting vertex corrections, for the diagonal part ($p0 = qj$) one simply gets,

$$\begin{aligned}&\widetilde{\sigma}^0_{\mu\mu}(\epsilon_1,\epsilon_2) = \\ &= (C/n)\sum_{p=1}^{n}\sum_{\alpha=A,B} c^\alpha_p \mathrm{tr}\left[\widetilde{J}^{p\alpha}_{\mu}(\epsilon_2,\epsilon_1)\widehat{\tau}^{pp}_{c}(\epsilon_1)J^{p\alpha}_{\mu}(\epsilon_1,\epsilon_2)\widehat{\tau}^{pp}_{c}(\epsilon_2)\right] \quad ,\end{aligned} \tag{12}$$

where

$$\widetilde{J}^{p\alpha}_{\mu}(\epsilon_2,\epsilon_1) = \widehat{D}^{pp}_{\alpha}(\epsilon_2)^t J^{p\alpha}_{\mu}(\epsilon_2,\epsilon_1)\widehat{D}^{pp}_{\alpha}(\epsilon_1) \quad . \tag{13}$$

Site-off-diagonal conductivity

The off-diagonal part can be partitioned into two terms

$$\widetilde{\sigma}^1_{\mu\mu}(\epsilon_1,\epsilon_2) = \widetilde{\sigma}^2_{\mu\mu}(\epsilon_1,\epsilon_2) + \widetilde{\sigma}^3_{\mu\mu}(\epsilon_1,\epsilon_2) \quad , \tag{14}$$

where

$$\widetilde{\sigma}^2_{\mu\mu}(\epsilon_1,\epsilon_2) = (C/n)\sum_{p=1}^{n}\sum_{q=1}^{n}(1-\delta_{pq}) \left\{\sum_{j\in I(L_2)} \mathrm{tr}\left\langle J^{p0}_{\mu}(\epsilon_2,\epsilon_1)\tau^{p0,qj}(\epsilon_1)J^{qj}_{\mu}(\epsilon_1,\epsilon_2)\tau^{qj,p0}(\epsilon_2)\right\rangle\right\} \quad , \tag{15}$$

and

$$\widetilde{\sigma}^3_{\mu\mu}(\epsilon_1,\epsilon_2) = (C/n)\sum_{p=1}^{n}\sum_{q=1}^{n}\delta_{pq} \left\{\sum_{(j\neq 0)\in I(L_2)} \mathrm{tr}\left\langle J^{p0}_{\mu}(\epsilon_2,\epsilon_1)\tau^{p0,qj}(\epsilon_1)J^{qj}_{\mu}(\epsilon_1,\epsilon_2)\tau^{qj,p0}(\epsilon_2)\right\rangle\right\} \quad . \tag{16}$$

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

$$\widetilde{\sigma}^2_{\mu\mu}(\epsilon_1,\epsilon_2) = (C/n)\left\{\sum_{p=1}^{n}\sum_{q=1}^{n}(1-\delta_{pq})\sum_{j\in I(L_2)}\sum_{\alpha,\beta=A,B} c^{\alpha}_{p}c^{\beta}_{q} \times \mathrm{tr}\left\{J^{p\alpha}_{\mu}(\epsilon_2,\epsilon_1)\left\langle\tau^{p0,qj}(\epsilon_1)J^{qj}_{\mu}(\epsilon_1,\epsilon_2)\tau^{qj,p0}(\epsilon_2)\right\rangle_{p0\alpha,qj\beta}\right\} \quad . \tag{17}$$

By employing the CPA condition and omitting vertex corrections (see Ref. [5]), $\widetilde{\sigma}^2_{\mu\mu}(\epsilon_1,\epsilon_2)$ is found to reduce to

$$\widetilde{\sigma}^2_{\mu\mu}(\epsilon_1,\epsilon_2) = (C/n)\left\{\sum_{p=1}^{n}\sum_{q=1}^{n}(1-\delta_{pq})\sum_{j\in I(L_2)}\sum_{\alpha,\beta=A,B} c^{\alpha}_{p}c^{\beta}_{q} \times \mathrm{tr}\left\{\widetilde{J}^{p\alpha}_{\mu}(\epsilon_2,\epsilon_1)\tau^{p0,qj}_{c}(\epsilon_1)\widetilde{J}^{q\beta}_{\mu}(\epsilon_1,\epsilon_2)\tau^{qj,p0}_{c}(\epsilon_2)\right\} \quad . \tag{18}$$

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

$$\tau^{p0,qj}_{c}(z) = \Omega^{-1}_{SBZ}\int e^{i\mathbf{k}\cdot\mathbf{R}_j}\hat{\tau}^{pq}(\mathbf{k},z)d^2k \quad , \tag{19}$$

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

$$\sum_{j\in I(L_2)}\tau^{p0,qj}_{c}(\epsilon_1)\tau^{qj,p0}_{c}(\epsilon_2) = \Omega^{-1}_{SBZ}\int\hat{\tau}^{pq}(\mathbf{k},\epsilon_1)\hat{\tau}^{qp}(\mathbf{k},\epsilon_2)d^2k \quad , \tag{20}$$

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

$$\widetilde{\sigma}^2_{\mu\mu}(\epsilon_1,\epsilon_2) = (C/n)\left\{\sum_{p=1}^{n}\sum_{q=1}^{n}(1-\delta_{pq})\,\Omega^{-1}_{SBZ}\sum_{\alpha,\beta=A,B} c^{\alpha}_{p}c^{\beta}_{q} \mathrm{tr}\int\left\{\widetilde{J}^{p\alpha}_{\mu}(\epsilon_2,\epsilon_1)\hat{\tau}^{pq}_{c}(\mathbf{k},\epsilon_1)\widetilde{J}^{q\beta}_{\mu}(\epsilon_1,\epsilon_2)\hat{\tau}^{qp}_{c}(\mathbf{k},\epsilon_2)d^2k\right\} \quad . \tag{21}$$

The last term in Eq. (14) to be evaluated is $\widetilde{\sigma}^3_{\mu\mu}(\epsilon_1,\epsilon_2)$ corresponding to the case that two sites are located in one and the same layer,

$$\widetilde{\sigma}^3_{\mu\mu}(\epsilon_1,\epsilon_2) = (C/n)\left\{\sum_{p=1}^{n}\Omega^{-1}_{SBZ}\sum_{\alpha,\beta=A,B} c^{\alpha}_{p}c^{\beta}_{p} \mathrm{tr}\int\widetilde{J}^{p\alpha}_{\mu}(\epsilon_2,\epsilon_1)\hat{\tau}^{pp}_{c}(\mathbf{k},\epsilon_1)\widetilde{J}^{p\beta}_{\mu}(\epsilon_1,\epsilon_2)\hat{\tau}^{pp}_{c}(\mathbf{k},\epsilon_2)d^2k\right\} + \widetilde{\sigma}^{3,corr}_{\mu\mu}(\epsilon_1,\epsilon_2) \quad , \tag{22}$$

where $\widetilde{\sigma}_{\mu\mu}^{3,corr}(\epsilon_1,\epsilon_2)$ arises from extending the sum to $\forall j \in I(L_2)$ and subtracting a corresponding correction term of the form

$$\begin{aligned}&\widetilde{\sigma}_{\mu\mu}^{3,corr}(\epsilon_1,\epsilon_2) = \\ &= -(C/n)\sum_{p=1}^{n}\sum_{\alpha,\beta=A,B} c_p^\alpha c_p^\beta \mathrm{tr}\left[\widetilde{J}_\mu^{p\alpha}(\epsilon_2,\epsilon_1)\widehat{\tau}_c^{pp}(\epsilon_1)\widetilde{J}_\mu^{p\beta}(\epsilon_1,\epsilon_2)\widehat{\tau}_c^{pp}(\epsilon_2)\right] \quad .\end{aligned} \tag{23}$$

Total conductivity for layered systems

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

$$\begin{aligned}&\widetilde{\sigma}_{\mu\mu}(\epsilon_1,\epsilon_2) = \\ &= (C/n)\sum_{p=1}^{n}\left\{\sum_{\alpha=A,B} c_p^\alpha \mathrm{tr}\left[\widetilde{J}_\mu^{p\alpha}(\epsilon_2,\epsilon_1)\widehat{\tau}_c^{pp}(\epsilon_1)J_\mu^{p\alpha}(\epsilon_1,\epsilon_2)\widehat{\tau}_c^{pp}(\epsilon_2)\right]\right. \\ &- \sum_{\alpha,\beta=A,B} c_p^\alpha c_p^\beta \mathrm{tr}\left[\widetilde{J}_\mu^{p\alpha}(\epsilon_2,\epsilon_1)\widehat{\tau}_c^{pp}(\epsilon_1)\widetilde{J}_\mu^{p\beta}(\epsilon_1,\epsilon_2)\widehat{\tau}_c^{pp}(\epsilon_2)\right] \\ &\left.+ \Omega_{SBZ}^{-1}\sum_{q=1}^{n}\sum_{\alpha,\beta=A,B} c_p^\alpha c_q^\beta \mathrm{tr}\int\left[\widetilde{J}_\mu^{p\alpha}(\epsilon_2,\epsilon_1)\widehat{\tau}_c^{pq}(\mathbf{k},\epsilon_1)\widetilde{J}_\mu^{q\beta}(\epsilon_1,\epsilon_2)\widehat{\tau}_c^{qp}(\mathbf{k},\epsilon_2)d^2k\right]\right\} \quad .\end{aligned} \tag{24}$$

Comparing the last equation with the corresponding bulk result [2],

$$\begin{aligned}&\widetilde{\sigma}_{\mu\mu}(\epsilon_1,\epsilon_2) = \\ &= (C/\Omega)\left\{\sum_{\alpha=A,B} c^\alpha \mathrm{tr}\left[\widetilde{J}_\mu^{\alpha}(\epsilon_2,\epsilon_1)\widehat{\tau}_c(\epsilon_1)J_\mu^{\alpha}(\epsilon_1,\epsilon_2)\widehat{\tau}_c(\epsilon_2)\right]\right. \\ &- \sum_{\alpha,\beta=A,B} c^\alpha c^\beta \mathrm{tr}\left[\widetilde{J}_\mu^{\alpha}(\epsilon_2,\epsilon_1)\widehat{\tau}_c(\epsilon_1)\widetilde{J}_\mu^{\beta}(\epsilon_1,\epsilon_2)\widehat{\tau}_c(\epsilon_2)\right] \\ &\left.+ \Omega_{BZ}^{-1}\sum_{\alpha,\beta=A,B} c^\alpha c^\beta \mathrm{tr}\int\left[\widetilde{J}_\mu^{\alpha}(\epsilon_2,\epsilon_1)\widehat{\tau}_c(\mathbf{k},\epsilon_1)\widetilde{J}_\mu^{\beta}(\epsilon_1,\epsilon_2)\widehat{\tau}_c(\mathbf{k},\epsilon_2)d^3k\right]\right\} \quad ,\end{aligned} \tag{25}$$

where Ω is the volume of the unit cell, 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, which is a direct consequence of the fact that in the growth direction of multilayers no translational invariance applies.

Defining finally layer-diagonal terms as

$$\begin{aligned}\widetilde{\sigma}_{\mu\mu}^{pp}(\epsilon_1,\epsilon_2) = \quad &(C/n)\sum_{\alpha=A,B} c_p^\alpha \left\{\mathrm{tr}\left[\widetilde{J}_\mu^{p\alpha}(\epsilon_2,\epsilon_1)\widehat{\tau}_c^{pp}(\epsilon_1)J_\mu^{p\alpha}(\epsilon_1,\epsilon_2)\widehat{\tau}_c^{pp}(\epsilon_2)\right]\right. \\ &\left.- \sum_{\beta=A,B} c_p^\beta \mathrm{tr}\left[\widetilde{J}_\mu^{p\alpha}(\epsilon_2,\epsilon_1)\widehat{\tau}_c^{pp}(\epsilon_1)\widetilde{J}_\mu^{p\beta}(\epsilon_1,\epsilon_2)\widehat{\tau}_c^{pp}(\epsilon_2)\right]\right\} \quad ,\end{aligned} \tag{26}$$

and layer-off-diagonal terms as

$$\begin{aligned}&\widetilde{\sigma}_{\mu\mu}^{pq}(\epsilon_1,\epsilon_2) = (C/n\Omega_{SBZ}) \\ &\quad\times\sum_{\alpha,\beta=A,B} c_p^\alpha c_q^\beta \mathrm{tr}\left[\int \widetilde{J}_\mu^{p\alpha}(\epsilon_2,\epsilon_1)\widehat{\tau}_c^{pq}(\mathbf{k},\epsilon_1)\widetilde{J}_\mu^{q\beta}(\epsilon_1,\epsilon_2)\widehat{\tau}_c^{qp}(\mathbf{k},\epsilon_2)d^2k\right] \quad ,\end{aligned} \tag{27}$$

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

$$\widetilde{\sigma}_{\mu\mu}(\epsilon_1,\epsilon_2) = \sum_{p=1}^{n}\left\{\widetilde{\sigma}_{\mu\mu}^{pp}(\epsilon_1,\epsilon_2) + \sum_{q=1}^{n}\widetilde{\sigma}_{\mu\mu}^{pq}(\epsilon_1,\epsilon_2)\right\} \quad . \tag{28}$$

Numerical applications

All calculations reported here are based on the fully relativistic spin-polarized Screened KKR method for generating the corresponding selfconsistent scattering potentials as well as for the evaluation of the electric conductivity tensor. In the former case a total of 45 $\mathbf{k}_{||}$ points in the irreducible wedge of the surface Brillouin zone is used, for the latter 1830 $\mathbf{k}_{||}$ points. The following systems were investigated as precursor cases for a study of the giant magnetoresistance in Co/Cu multilayers

Substrate	Cu(100)
Multilayer	$(\mathrm{Cu})_n \quad , n = 1, 45$
Cap	Cu(100)

Substrate	Cu(100)
Multilayer	$(\mathrm{Co})_n \quad , n = 1, 39$
Cap	Cu(100)

Substrate	Cu(100)
Multilayer	$(\mathrm{Cu}_{0.85}\mathrm{Co}_{0.15})_n \quad , n = 1, 30$
Cap	Cu(100)

As is well-known from bulk theory, (at zero temperature) for fcc Cu the resistance is exactly zero, whereby for the tensor elements the relation

$$\rho_{xx} = \rho_{yy} = \rho_{zz}$$

applies. Quite clearly by using Eq. (28) this will only be the case if the number of layers to be summed over is sufficiently large, a fact, which of course supplies an excellent test of the applied numerical means.

In Figure 1 the resistivities $\rho_{xx}(= \rho_{yy})$ and ρ_{zz} ($\rho_{\mu\mu} = 1/\sigma_{\mu\mu}$) are shown as a function of the number of layers of Cu on top of a Cu(100) substrate and capped semi-infinitely by Cu(100). Since $n\rho_{\mu\mu}$ shows a linear behavior with respect to n (for sufficiently large n) the curves can be extrapolated to very large n. As one can see in this Figure ρ_{xx} and ρ_{zz} indeed go exactly to zero as in Eq. (28) the number of layers increases. In addition, for a large enough number of layers one loosely could state that cubic symmetry is "restored".

In order to understand this Figure and also the following ones properly, it is necessary to recall that this reflects nothing but the fact that as compared to the bulk expression Eq. (25) in Eq. (28) the "missing" lattice Fourier transformation in one direction, namely in direction of the surface normal, shows up as a finite sum. In principle, therefore, only as n approaches the order of the translational group for translations along the surface normal, a bulk-like result can be expected. This has important consequences for realistic multilayer systems, in which the number of layers can be rather small: "confinement" effects apply in such systems and even for a system with growth direction (100) in general

$$\rho_{xx} \neq \rho_{zz} \quad .$$

It is very reassuring that the numerical procedures applied indeed show the correct behavior discussed above (as n becomes very large).

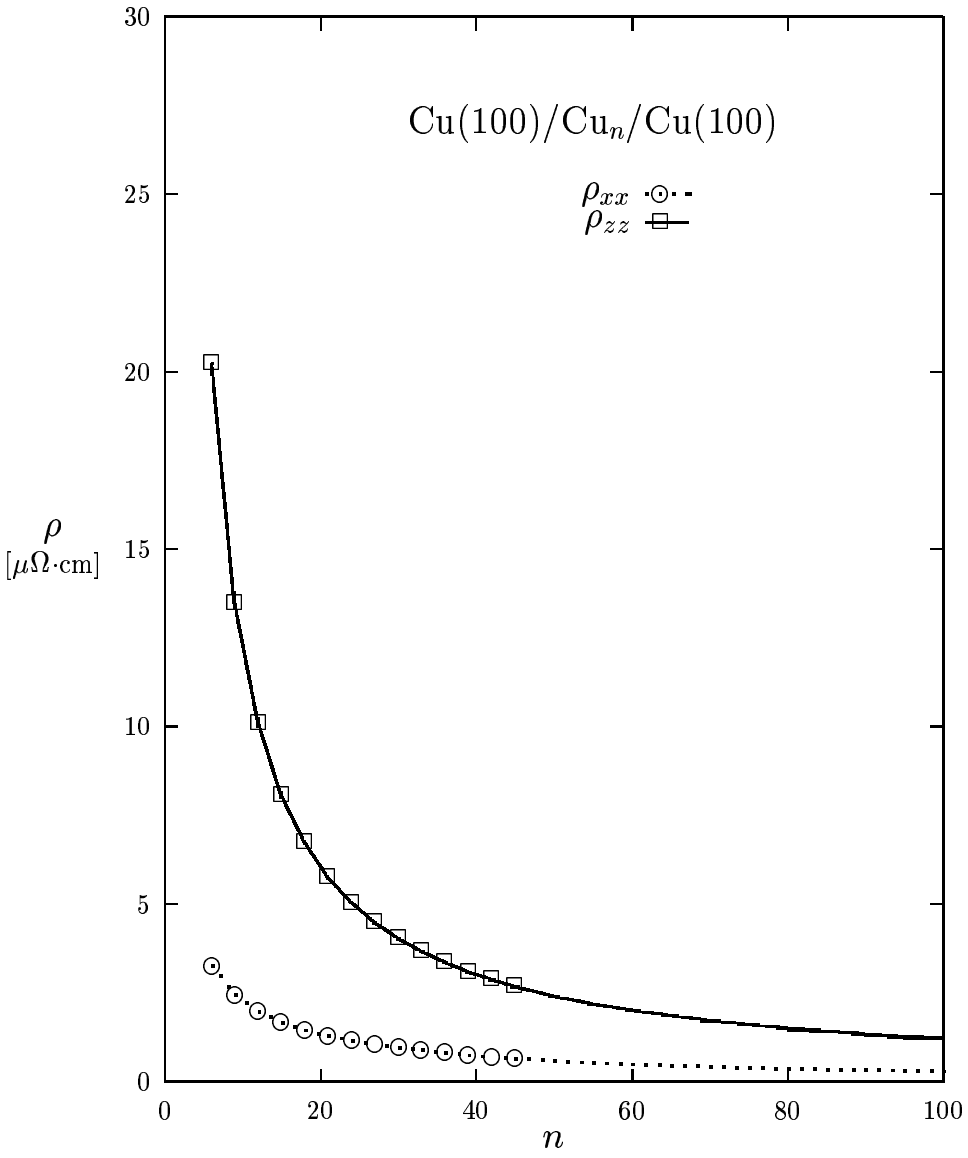

Figure 1: $\rho_{xx}(=\rho_{yy})$ and ρ_{zz} for Cu(100)/Cu$_n$/Cu(100) as a function of the number of Cu-layers n. The symbols mark the n-values for which the calculations were performed, the lines refer to the extrapolation for large n (see discussion in the text).

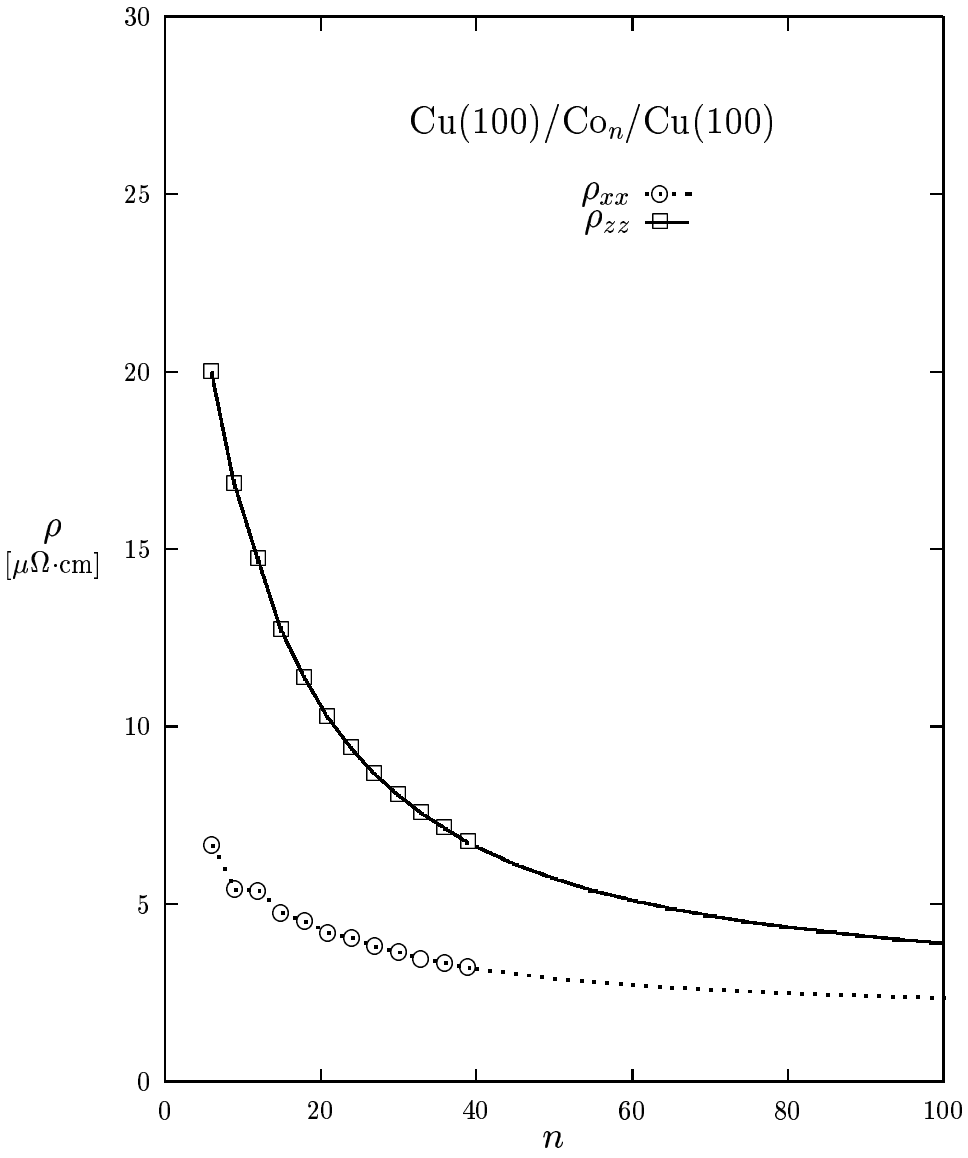

Figure 2: $\rho_{xx}(=\rho_{yy})$ and ρ_{zz} for Cu(100)/Co$_n$/Cu(100) as a function of the number of Co-layers n. The symbols mark the n-values for which the calculations were performed, the lines refer to the extrapolation for large n (see discussion in the text).

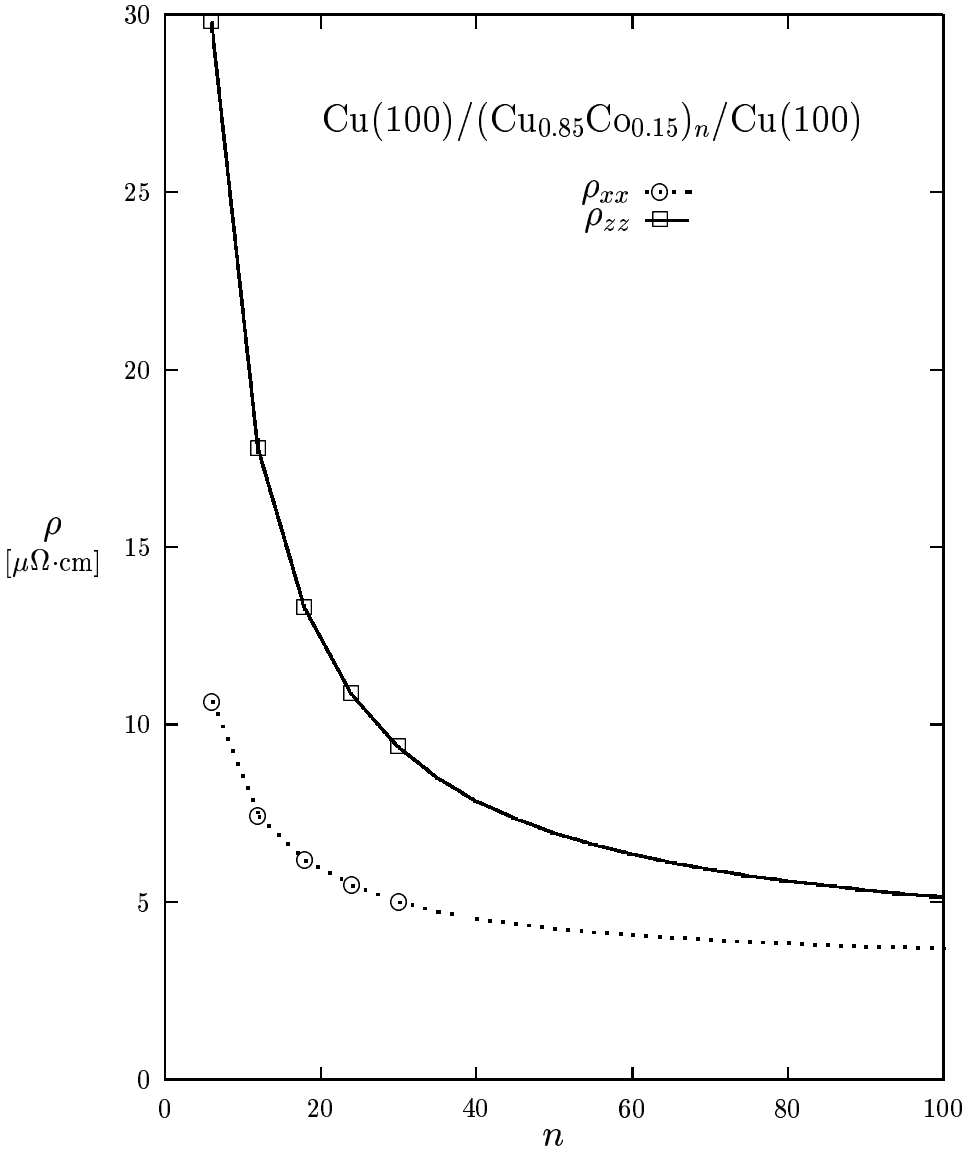

Figure 3: $\rho_{xx}(=\rho_{yy})$ and ρ_{zz} for Cu(100)/$(Cu_{0.85}Co_{0.15})_n$/Cu(100) as a function of the number of $(Cu_{0.85}Co_{0.15})$-layers n. The symbols mark the n-values for which the calculations were performed, the lines refer to the extrapolation for large n (see discussion in the text).

In Figures 2 and 3 the same type of display is shown when the multilayer consists of a finite number of Co-layers and a finite number of statistically disordered ($Cu_{0.85}Co_{0.15}$) layers, respectively. In these two cases as the number of layers increases the resistivities cannot approach zero, but have to tend to a constant. As one can see this is indeed the case. In the case of pure Co layers one could call this constant a "contact" contribution to the resistivity. For the alloy case it is interesting to observe, that for large enough n the resistivity is of the same order of magnitude that characterizes the resistivity of noble metal rich alloys with transition metals. Of course the constant obtained and to be seen in Figure 3 is not quite the resistivity for a bulk alloy of fcc $Cu_{0.85}Co_{0.15}$ since (a) the lattice constant and the Fermi energy of pure Cu apply and (b) the meaning of a "contact" resistivity pertains. Only in the case that the (semi-infinite) substrate and the (semi-infinite) cap are of the same material – $Cu_{0.85}Co_{0.15}$ in the present example – the resistivity for large enough n picks up the meaning of a residual resistivity. It should be noted that even though the present examples are meant to serve as numerical tests, it is evident that such systems very well can serve as example for an ab-initio calculation of "contact" resistivities which otherwise are computationally inaccessible.

Presently the method and numerical techniques illustrated in this contribution are applied to a study of the giant magnetoresistance (GMR) in Co/Cu multilayer systems and also for studying the effect of repetitions ("repeats") of multilayers as is the case in most experimental systems on the GMR.

Acknowledgement

This paper was supported by the Austrian Science foundation (P11266), the TMR network on *Ab initio calculations of magnetic properties of surfaces, interfaces and multilayers* (Contract No. EMRX-CT96-0089) and has benefited from collaborations within the HCM network Contract No. ERBCHRXCT930369.

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