

# First Principles Calculation of Electrical Conductivity and Giant Magnetoresistance of Co|Cu Multilayers

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## ABSTRACT

We show that the Kubo formula can be used to calculate the non-local electrical conductivity of layered systems from first principles. We use the Layer Korringa Kohn Rostoker method to calculate the electronic structure and the Green function of Co|Cu|Co trilayers within the local density approximation to density functional theory. This Green function is used to calculate the conductivity through the Kubo formula for both majority and minority spins and for alignment and anti-alignment of the Co moments on either side of the Cu spacer layer. This allows us to determine the giant magnetoresistance from first principles. We investigate three possibilities for the scattering in Co|Cu|Co: (1) equal electron lifetimes for Cu, majority spin Co, and minority spin Co, (2) equal electron lifetimes for majority and minority Co, weaker scattering in Cu and spin dependent interfacial scattering, (3) electron lifetimes for majority and minority spin cobalt proportional to their Fermi energy densities of states and spin dependent interfacial scattering.

## Introduction

Recently there has been great interest in the transport properties of layered magnetic materials because of the discovery of a new form of magnetoresistance[1, 2] called the giant magnetoresistance (GMR). GMR is a change (generally a pronounced decrease) in the electrical resistance of an inhomogeneous system that is observed when an applied magnetic field causes an alignment of the magnetic moments in different parts of the material. GMR has been observed in several geometries, but the most promising and interesting GMR systems are composed of thin layers of ferromagnetic material separated by non-magnetic or very weakly magnetic spacer layers.

The transport properties of layered materials have been the subject of several theoretical investigations based on the model of free electrons with random point scatterers (FERPS). Using this model, Fuchs[3] and later Sondheimer[4] obtained a solution to the semi-classical Boltzmann equation with boundary conditions appropriate to free electrons in a thin film. Barnás and coworkers[5] extended this approach to the case in which the film has several layers with differing scattering rates. Levy and coworkers[6, 7, 8, 9, 10] applied the more rigorous Kubo-Greenwood[11, 12] formula to the FERPS model and developed two different approximations for transport in magnetic multilayers. Zhang and Butler[13] have recently evaluated the Kubo-Greenwood formula exactly for the FERPS model applied to multilayers. Their results allow a comparison of the relative success of the various approximations in representing the conductivity of the free electron model. They found that the semi-classical

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approximation works surprisingly well for the FERPS model applied to multilayers.

In addition to theoretical treatments of GMR based on the FERPS model there have been a few previous applications of first principles techniques. Butler, *et. al.*[14] calculated the GMR for periodic multilayers of copper and cobalt and of copper and permalloy ( $\text{Ni}_{0.8}\text{Fe}_{0.2}$ ). They calculated the complex energy bands using the coherent potential approximation and showed that the imaginary part of the crystal momentum can be interpreted as the inverse of twice the electron mean free path. Their calculations showed that there is the potential for a very large GMR due to spin dependent interfacial scattering because the Fermi energy scattering amplitudes for majority spin cobalt, majority spin nickel and majority spin iron (as an impurity in nickel) are all very similar. Nesbet[15] reached a similar conclusion in studies of periodic  $\text{Cu}_2\text{Co}$  multilayers. Schep *et. al.*[16] have investigated a very different form of GMR from that seen experimentally by assuming that electron transport is *ballistic* rather than diffusive.

In this paper we report on first-principles calculations of the electronic structure of cobalt-copper multilayers. Using this electronic structure we calculate the conductivity by evaluating the Kubo-Greenwood linear response formula. We do not assume that the scattering is weak or that the electron wave functions are those of free electrons nor do we make the semi-classical approximations necessary to apply Boltzmann theory. It should also be noted that our approach does not require periodicity perpendicular to the layers so that it can be applied to spin valves and trilayers.

## Conductivity of Inhomogeneous Systems

We define the nonlocal conductivity  $\sigma_{\mu\nu}^s(\mathbf{r}, \mathbf{r}')$  as the linear response of the current of electrons of spin  $s$  at point  $\mathbf{r}$  in direction  $\mu$  to the local applied field at point  $\mathbf{r}'$  in direction  $\nu$ ,

$$J_{\mu}^s(\mathbf{r}) = \int d\mathbf{r}' \sum_{\nu} \sigma_{\mu\nu}^s(\mathbf{r}, \mathbf{r}') E_{\nu}^s(\mathbf{r}'). \quad (1)$$

Here "local applied field" means the change in the local electrostatic field that arises due to the application of a potential difference across the sample. For an inhomogeneous system this may differ from the average applied field and it may be different for different spins[8].

For a homogeneous system, the current and applied field can be assumed to be uniform so that one can define a single conductivity which is also uniform,  $J_{\mu}^s = \sum_{\nu} \sigma_{\mu\nu}^s E_{\nu}$ . This is the conductivity which is given by the Kubo-Greenwood formula[11, 12],

$$\sigma_{\mu\nu}^s = \frac{\pi\hbar}{N\Omega} \left\langle \sum_{\alpha, \alpha'} \langle \alpha | j_{\mu} | \alpha' \rangle \langle \alpha' | j_{\nu} | \alpha \rangle \delta(\epsilon_F - \epsilon_{\alpha}) \delta(\epsilon_F - \epsilon_{\alpha'}) \right\rangle \quad (2)$$

where  $j_{\mu}$  is the current operator,  $j_{\mu} \equiv (-i\hbar e/m_e)\partial/\partial r_{\mu}$ ,  $\Omega$  is the volume per atom and  $N$  is the number of atoms. The quantum states  $|\alpha\rangle$  in Eq. (2) represent the exact eigenfunctions of a particular configuration of the random potential, and the large angle brackets indicate an average over configurations.

In order to define a non-local site dependent conductivity,  $\sigma_{\mu\nu}^{i,j,s}$ , we define the current density at site  $i$  for spin  $s$  as the average of the current density over the atomic cell at that site,  $J_{\mu}^{i,s} = \Omega_i^{-1} \int_{\Omega_i} d\mathbf{r} J_{\mu}^s(\mathbf{r})$ . We also assume that the local field,  $E_{\nu}^s(\mathbf{r})$ , is constant over each atomic cell. Thus we write Ohm's law in a discrete form in which the current at site  $i$  is

related to the local electric field at site  $j$  through the two point conductivity function,  $\sigma^{ij}$ ,

$$J_\mu^{i,s} = \sum_{j\nu} \sigma_{\mu\nu}^{ij,s} E_\nu^{j,s}. \quad (3)$$

The superscript  $s$  on the local field indicates that it can be spin dependent. The local field will be determined *after* the non-local conductivity is determined by the requirement of current continuity in the steady state,  $\sum_\mu \partial J_\mu^s(\mathbf{r})/\partial r_\mu = 0$ .

The intersite conductivity,  $\sigma_{\mu\nu}^{ij,s}$ , is given by Eq.(2) with the matrix element integrals  $\langle \alpha | j_\mu | \alpha' \rangle$  and  $\langle \alpha' | j_\nu | \alpha \rangle$  restricted to sites  $i$  and  $j$  respectively and can be seen to depend on the *imaginary part* of the Green function,  $\sum_\alpha |\alpha\rangle \langle \alpha| \delta(\epsilon_F - \epsilon_\alpha)$ . It can be written in terms of the Green function,  $G(\mathbf{r}, \mathbf{r}'; \epsilon_F)$ , by writing,

$$\sigma_{\mu\nu}^{ij,s} = \frac{1}{4} \sum_{p,p'=\pm 1} (pp') \tilde{\sigma}_{\mu\nu}^{ij,s}(\epsilon_F + i\eta p, \epsilon_F + i\eta p'), \quad (4)$$

where  $\eta$  is infinitesimal and where

$$\tilde{\sigma}_{\mu\nu}^{ij,s}(z_1, z_2) = \frac{-\hbar}{\pi \Omega_i} \int_{\Omega_i} d\mathbf{r} \int_{\Omega_j} d\mathbf{r}' \langle j_\mu(\mathbf{r}) G^s(\mathbf{r}, \mathbf{r}'; z_1) j_\nu(\mathbf{r}') G^s(\mathbf{r}', \mathbf{r}; z_2) \rangle. \quad (5)$$

Following[17] we can write the Green function in terms of the scattering path operator of multiple scattering theory, and the local solutions to the Schrödinger equation. These are determined by the atomic potentials which are obtained self-consistently by using the local spin density approximation to density functional theory. For the case in which the only scattering is due to impurities or to alloying one can use the Coherent Potential Approximation to average the two particle Green function[18]. In this paper we shall take a simpler and more general approach. In realistic GMR systems the scattering usually comes from several sources: impurities, grain boundaries, vacancies, voids, static displacements, phonons, static moment misalignment and magnons. The proper first principles treatment of any one of these scattering mechanisms is quite tedious and the simultaneous treatment of all of them would be difficult and probably pointless since we do not have a sufficiently detailed characterization of experimental GMR systems to know the strengths, concentrations and other relevant parameters of these defects. In this paper we approximate the scattering processes by a phenomenological local scattering rate. Thus we average the two Green functions independently and assume that the effect of this averaging is that each atomic potential acquires an imaginary term which describes the scattering rate in its vicinity.

## Application to Layered Systems

We now consider the special case of layered systems. We assume that the system has a two dimensional periodicity, but that its properties may vary in the third dimension. Thus different atomic layers may consist of different types of atoms and have different concentrations of impurities, but there is a common periodicity to all of the layers after averaging over impurity configurations. We use a notation in which a site labeled by  $i$  in the preceding section and representing any lattice site in the three dimensional crystal acquires two labels  $i \rightarrow Ii$ , where the upper case  $I$  distinguishes different *atomic* layers and the lower case  $i$  labels a site within layer  $I$ . The interlayer conductivity can then be written in the form  $\tilde{\sigma}^{IJ} = N_I^{-1} \sum_{ij} \tilde{\sigma}^{IiJj}$ , where  $N_I$  is the number of atoms per layer.

Because of the two dimensional periodicity we can relate the Green function which connects any two sites  $G^{IiJj}$  to a Green function which connects layers through an integral over the two dimensional Brillouin zone, of area  $\Omega_z$ .

$$G^{IiJj} = \Omega_z^{-1} \int_{\Omega_x} d^2 \mathbf{q} G^{IJ}(\mathbf{q}) e^{i\mathbf{q}\cdot(\mathbf{R}_i - \mathbf{R}_j)}. \quad (6)$$

These layer Green functions  $G^{IJ}$  can be calculated using the layer KKR formalism[19]. The final expression for the conductivity is expressed in terms of matrices indexed by the layer numbers,

$$\tilde{\sigma}_{\mu\nu}^{IJ} = \Omega_z^{-1} \int_{\Omega_x} d^2 \mathbf{q} M_{\mu}^I G^{IJ}(\mathbf{q}) M_{\nu}^J G^{JI}(\mathbf{q}) \quad (7)$$

where  $M_{\mu}^I$  represents a dipole matrix element in direction  $\mu$  evaluated for a site in layer  $I$ . Details of the conductivity formalism will be given elsewhere[20].

The local fields can be determined after  $\sigma^{IJ_s}$  is obtained by using  $J^{I_s} = \sum_K \sigma^{IK_s} E^{K_s}$  and the condition that the current for each spin must be continuous in the steady state. Two geometries are commonly discussed. If the field is applied parallel to the layers, a geometry sometimes referred to as ‘‘CIP’’ for ‘‘current in the plane’’, the local fields will be uniform by symmetry and equal to the average applied field. Thus the overall conductivity will be given by  $\sigma = d^{-1} \sum_{IK_s} d_I \sigma^{IK_s}$  where  $d_I$  is the thickness of layer  $I$ , and  $d$  is the total film thickness. If the field is applied perpendicular to the layers, a geometry referred to as ‘‘CPP’’ for current perpendicular to the planes, then  $J^{I_s}$ , will be independent of  $I$  for each spin. Thus  $J^s = \sum_K \sigma^{IK_s} E^{K_s}$  and the local fields can be obtained (at least in principle) by inverting  $\sigma^{IK_s}$ ,

$$E^{I_s} = \sum_K [(\sigma^s)^{-1}]^{IK} J^s = \sum_K \rho_s^{IK} J^s. \quad (8)$$

## Non-Local Conductivity of Free Electrons, Copper, and Cobalt

It is important to understand the non-local conductivity if one wants to understand GMR because it is the non-local nature of the conductivity that leads to GMR. We shall see that the form of the non-local conductivity is a fairly sensitive function of the electronic structure.

We used Eq.(7) to calculate the non-local electrical conductivity for free electrons, for copper and for cobalt using various values for the scattering rate,  $\Delta = \hbar/\tau$ . Figure 1 shows the non-local layer dependent conductivities for free electrons calculated using our first principles codes compared with exact results from the analytic formulas obtained by Zhang and Butler[13]. The atomic layers were taken to be perpendicular to the (111) direction. These calculations assumed a scattering rate,  $\Delta = \hbar/\tau$  of 0.01 Hartree (0.272 eV), one electron per atom, and a lattice constant appropriate to copper (6.8165 Bohr). They were performed as a check of the first-principles code, the validity of approximating the atomic cells by spheres, and the degree of convergence of the integration over the two dimensional Fermi surface.

The agreement is quite satisfactory. We believe that most of the small discrepancy between the analytic and first principles results actually arises from a small difference in the way the spatial averages over layers  $I$  and  $J$  are performed in the two cases. The first-principles  $\sigma^{IJ}$  involves volume averages of the microscopic non-local conductivity  $\sigma(\mathbf{r}, \mathbf{r}')$  over the atomic cells (here approximated by spheres) in layers  $I$  and  $J$ . For the analytic free electron results, however, the averages are over slabs with a thickness equal to the interlayer spacing and bounded by planes perpendicular to the  $z$  axis.

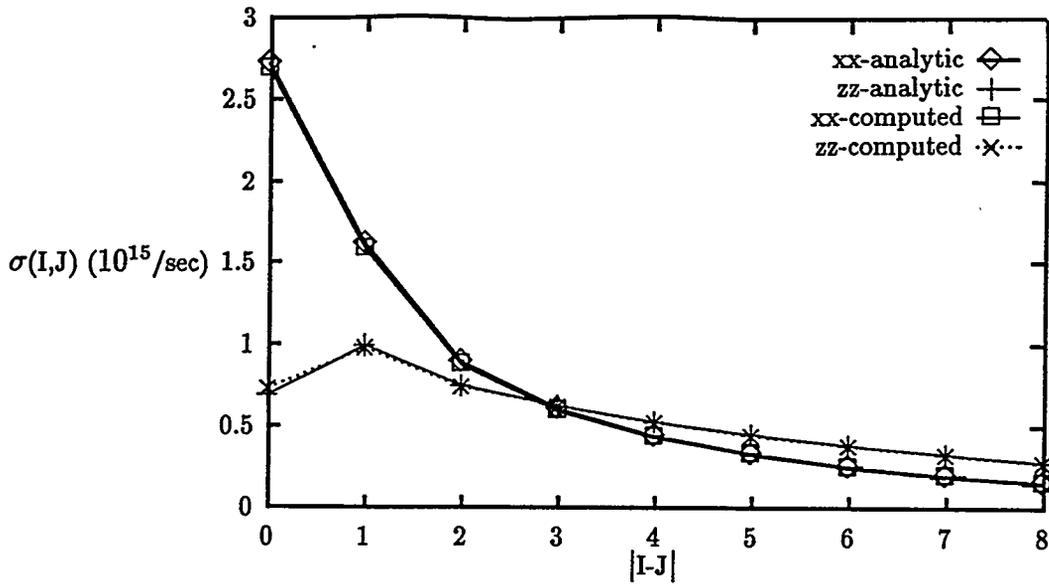


Figure 1: Non-local layer dependent conductivity for free electrons. Diamonds ( $\diamond$ ) and squares ( $\square$ ) represent exact analytic results and results calculated using the first-principles code, respectively for CIP. Pluses (+) and crosses ( $\times$ ) represent exact analytic and first-principles results respectively for CPP. The analytic results are averaged over a slab with the thickness of an atomic layer. The first principles results are averaged over the atomic spheres in a plane. The Fermi Energy is 0.2595 Hartrees.

Figure 2 shows the calculated values of the non-local layer dependent conductivity,  $\sigma_{\mu\nu}^{IJ}$ , for copper and for cobalt at their respective Fermi energies using a scattering rate of 0.005 Hartree (0.136 eV). The atomic planes were again taken to be perpendicular to the (111) direction. In addition to the calculated non-local conductivities we show attempts to fit these results with the free electron model. For copper, one can obtain a reasonable fit to the non-local conductivity both parallel to the planes,  $\sigma_{xx}^{IJ}$ , and perpendicular to them,  $\sigma_{zz}^{IJ}$ . The fit shown assumes that the Fermi energy is appropriate to one electron per atom (0.26 Hartree) and the effective mass is 1.52 times the free electron mass.

Figure 2 also shows the non-local layer dependent conductivities for majority and minority spin cobalt. The majority spin conductivity was fit to the free electron results using an effective Fermi energy of 0.111 Hartree which agrees qualitatively with a model for majority carriers in cobalt which assumes that the Fermi surface for the majority spins contains less than 0.5 electrons. The scattering rate used in the fit was 0.0046 Hartree. The fit works well for large values of  $|I - J|$  but significantly underestimates the conductivity for small values. This can be interpreted as indicating the presence of two types of majority spin cobalt electrons. One type has a relatively short mean free path. The other type has a longer mean free path and fits reasonably well to the free electron model. Also shown is the non-local conductivity of minority spin cobalt. Note that these data points have been multiplied by 0.1 to shift them downwards on the plot. We were unable to obtain a good fit to the free electron model for this data. The free electron model will need to be extended, e.g. by having at least two kinds of carriers, in order to represent the calculated non-local conductivity of minority spin cobalt. It should be noted that the current carried by the minority electrons is not negligible.

The results for cobalt illustrate the difficulty associated with applying free electron models

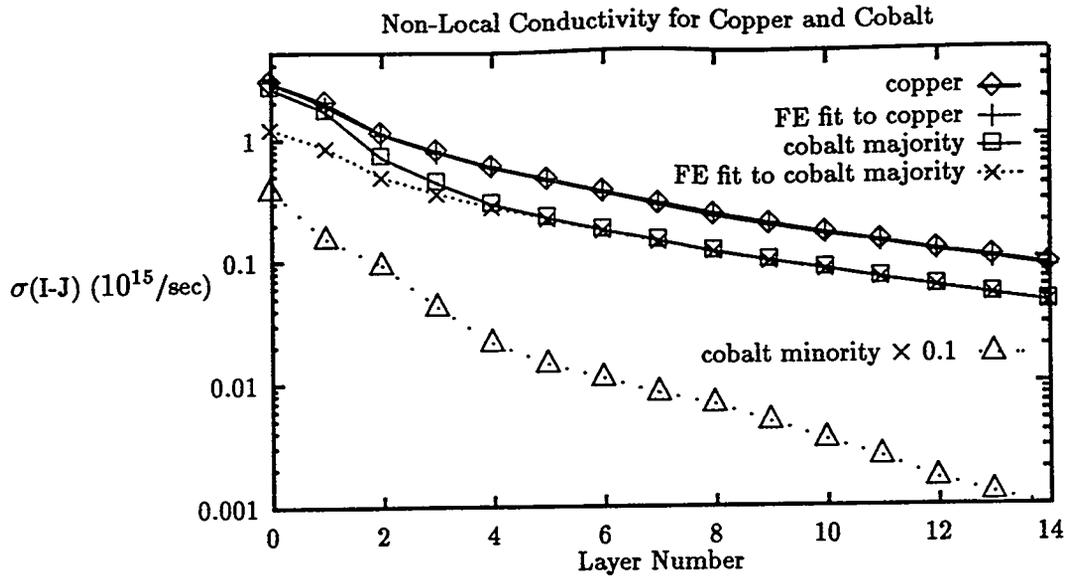


Figure 2: Non-local layer dependent conductivity for copper and cobalt. Diamonds ( $\diamond$ ) represent the non-local conductivity for copper, pluses (+) a free-electron fit. Squares ( $\square$ ) represent the non-local conductivity for majority cobalt, crosses ( $\times$ ) a free-electron fit. Triangles ( $\triangle$ ) represent cobalt minority.

to transition metals. The assumption of the same lifetime for both the majority and minority spins yields, according to our calculations, very nearly the same conductivities for the two channels, *e.g.* for a scattering rate  $\hbar/\tau$  of 0.005 Hartrees we calculate a single channel majority spin resistivity of  $58.5 \mu\Omega\text{cm}$  and a minority spin resistivity of  $60.8 \mu\Omega\text{cm}$ . It is clear, however, that the mean free paths are very different for the two channels and that for minority spin cobalt one needs at least two mean free paths to represent the non-local conductivity. This is consistent with our knowledge of d-band metals. The Fermi velocity can vary by large factors over the Fermi surface. Typically the flat portions of the bands contribute strongly to the density of states and they can also contribute moderately to the conductivity but the contribution will be relatively local in nature. The more dispersive portions of the Fermi surface contribute weakly to the density of states but contribute significantly to the conductivity and especially to the non-local conductivity.

### Electronic Structure of Copper layers embedded in Cobalt

As a model of the electronic structure of a Co|Cu|Co trilayer we calculated the self-consistent electronic structure of cobalt at its experimental lattice constant. Then we inserted differing numbers of interface cobalt and copper layers into the bulk cobalt, and again solved the electronic structure self-consistently holding the Fermi energy fixed at that of bulk cobalt. We used the Green function technique so that we could treat an infinite system without the need of assuming artificial periodicities. The largest system that we treated had 24 (111) atomic layers that were calculated self-consistently: 7 cobalt followed by 10 copper followed by 7 cobalt. These 24 layers were embedded in an infinite matrix of self-consistently determined cobalt (111) atomic layers.

The calculated charge on each of the layers is shown in Fig. 3. The net charge transfer

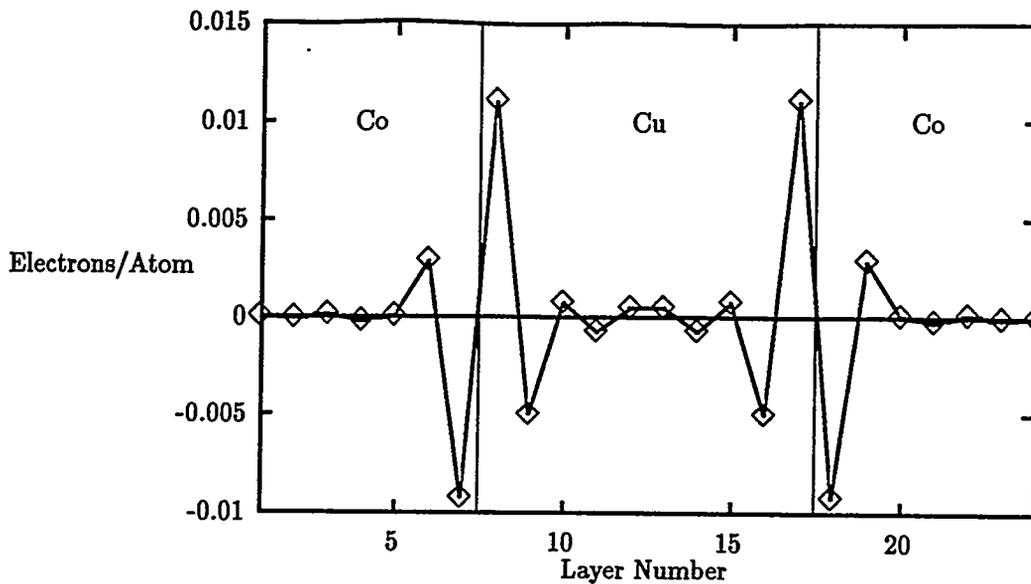


Figure 3: Calculated charge on each layer.

between cobalt and copper is quite small. We calculate that approximately .01 electrons are transferred to the copper, but this number might change slightly if the lattice were relaxed. In these calculations the copper has the same lattice spacing as cobalt. We neglected the small (2%) difference between the lattice constants of bulk cobalt and bulk copper. We also calculated the self-consistent moments and charges for the anti-parallel arrangement of the cobalt moments. The change in the charges and in the magnitude of the moments between the parallel and anti-parallel alignments was less than .001 electrons for every layer.

Figure 4 shows how the valence electrons are divided between the majority and minority spin channels. Note that there is a reasonably close match between the majority Co and the Cu in terms of the number of electrons per atom. The number of valence electrons on the Cu and Co sites differ by less than 0.2 electrons. For the minority spin electrons on the other hand the difference is much larger, more than 1.8 electrons. To a good approximation the electronic structure of ideal Co|Cu interfaces can be understood in terms of a very simple picture. First, there is very little charge transfer between the Co and the Cu. Second, the moment changes are relatively small near the interfaces so that Co moments are all around 1.7 Bohr magnetons. The consequence of this is that the number of valence electrons per atom per spin channel is 5.5 for Cu and approximately 5.35 for majority spin Co and 3.65 for minority spin cobalt.

This approximate "matching" of the number of valence electrons per atom in the majority spin channel means that the atomic cobalt and copper potentials appear very similar to majority spin electrons. This can be verified by considering the scattering phase shifts for electrons at the Fermi energy. These are very similar for copper majority cobalt, but differ greatly for copper and cobalt minority, particularly for the *d*-phase shifts which because of the large *d* Fermi energy density of states and the large magnitude of the phase shifts are the primary determinants of the scattering. Another important qualitative difference between the majority and minority spin channels is a large difference in the Fermi energy density of states on the cobalt layers. The Fermi Energy DOS for the minority spin channel is approximately 7.34 times as large as for the majority channel for the cobalt layers.

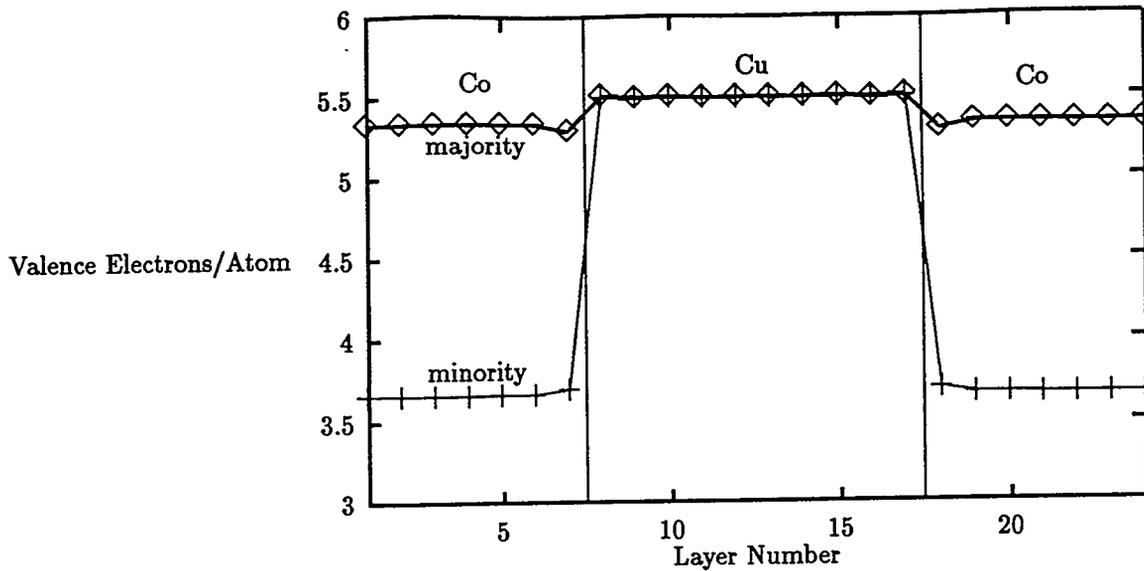


Figure 4: Calculated numbers of majority and minority valence electrons per atom for each layer.

### Non-Local Conductivities Near Interfaces

Figure 5 shows calculated non-local layer dependent conductivities for 10 layers of copper embedded in cobalt. This figure shows the conductivity for currents in the plane of the layers, the usual experimental geometry. For this calculation, we assumed the same lifetime,  $\hbar/\tau = 0.005$  Hartrees, for the copper layers as for the cobalt layers. Because the majority spin cobalt potential “matches” that of the copper, the non-local layer dependent conductivity for the Co|Cu|Co trilayer in the majority spin channel (Fig. 5a) is very similar to that of pure cobalt (majority spin) or pure copper. The major difference being that the local conductivity is reduced for the copper layer at the interface.

For the minority spin electrons, however, the interfaces greatly modify the conductivities as is shown in Fig. 5b. The conductivities of the copper layers near the interface are greatly reduced. Those on the cobalt layers near the interface are also affected. The local conductivity (peak at  $I = J$ ) is enhanced but the non-local contributions drop off much faster as a function of distance.

The calculated conductivity for anti-parallel alignment for the majority spin channel (relative to the left hand side of the film) is shown in Fig. 5c. These calculations were based on electronic structures calculated self-consistently for the anti-parallel alignment. As might be expected the conductivities on the left hand side appear similar to those of the majority channel for parallel alignment and those on the right hand side appear similar to those of the minority spin for parallel alignment. The conductivity for the other spin channel is identical except reversed left to right.

The difference between the total conductivities for the two alignments is the GMR or more precisely the giant magnetoconductance and is shown in Fig. 5d. The contributions to the giant magnetoconductance are seen to arise from completely different regions than the major contributions to the conductivity. The highest peaks correspond to currents flowing in cobalt layers (I) at one interface which sense the field in the cobalt layer (J) at the other interface. There is also a “ridge” of contributions running through the copper, i.e. currents

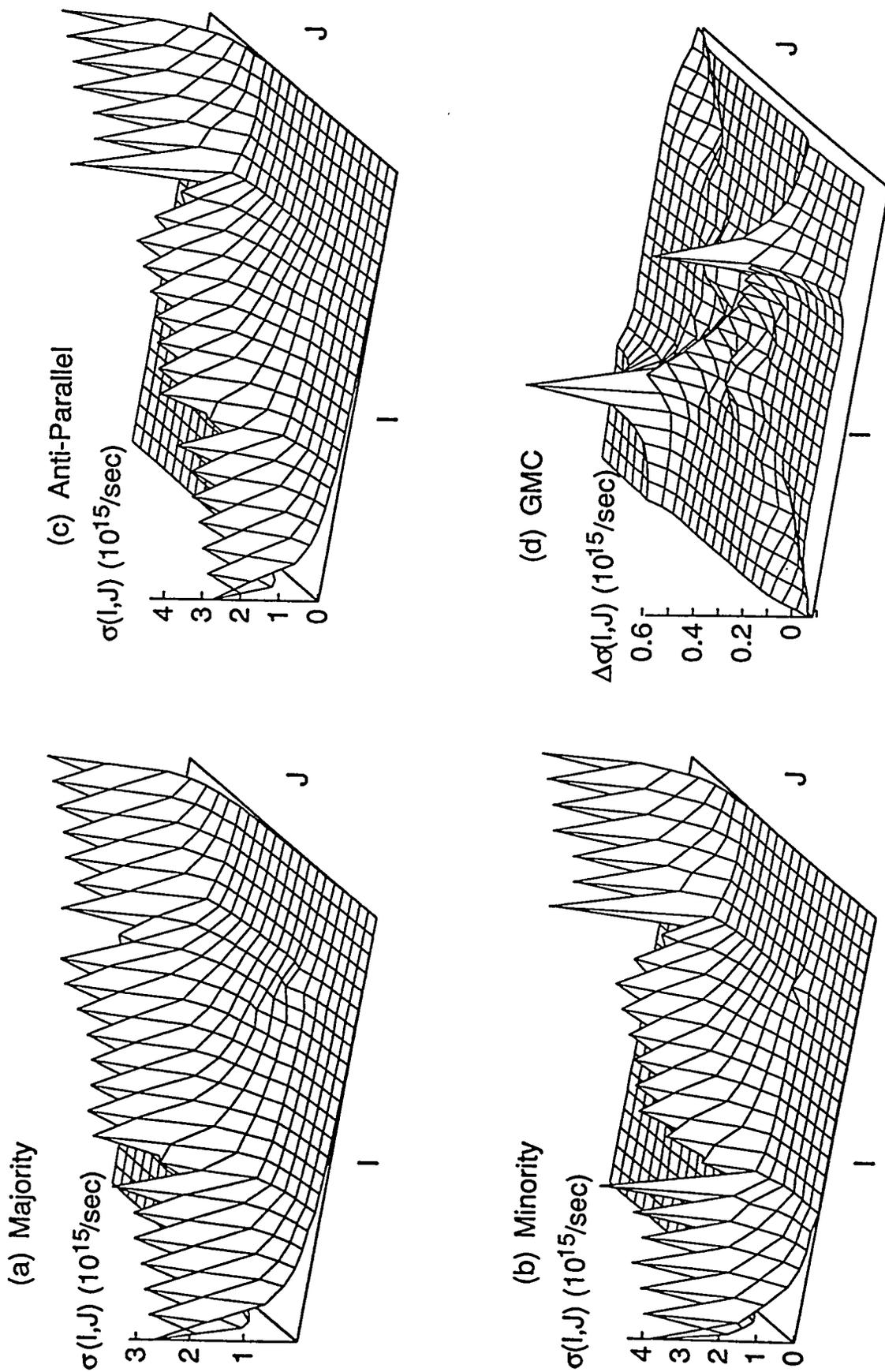


Figure 5: Non-local layer dependent conductivities for 10 layers of copper embedded in cobalt. A scattering rate of 0.005 Hartrees was assumed for all layers.

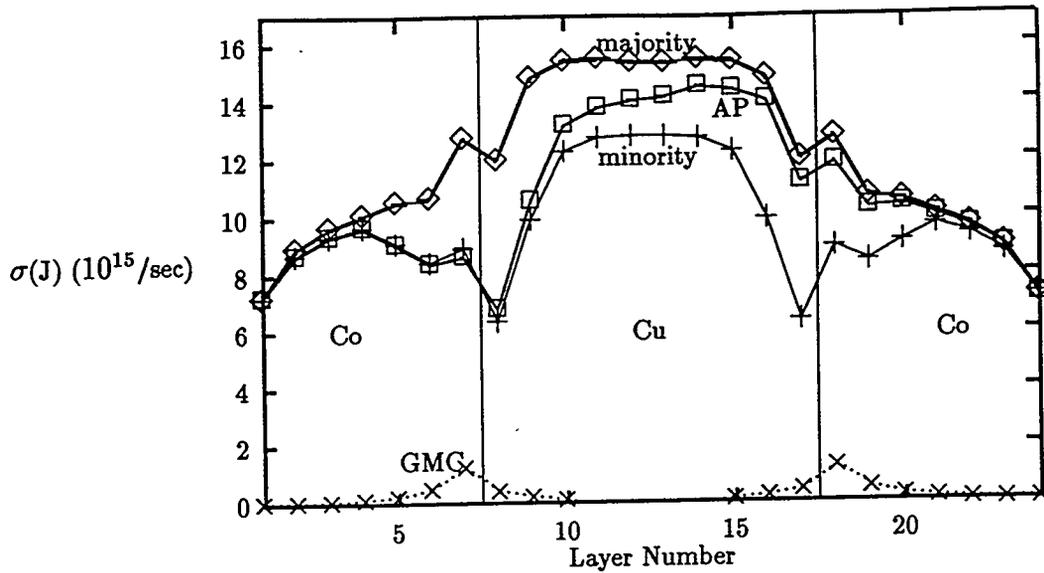


Figure 6: Layer dependent conductivities corresponding to the non-local layer dependent conductivities of Figure 5.

flowing in one copper layer due to fields sensed in its mirror image layer on the other side of the interface. There is also a region of slightly negative magnetoconductance for  $I \approx J$  in the cobalt layers.

Figure 6 shows layer dependent conductivities, *i.e.* the sum over  $I$  or  $J$  of  $\sigma(I, J)$ . It can be seen that the assumption of equal lifetimes for all layers leads to a small GMR and that the magnetoconductance flows mainly in the cobalt layers adjacent to the interface. One can also gain an insight into the origin of the GMR by noting how the anti-parallel (AP) conductivity varies with layer number. Note that we have plotted the conductivity of only one of AP channels because the other is its mirror image. On the left hand side of the figure for which the plotted AP spin channel is locally the minority, the AP conductivity is almost identical to the minority conductivity. On the right hand side, however, where the plotted AP channel is locally the majority, the AP conductivity is less than the majority. It is this difference that causes the GMR. The majority and AP currents on the right hand side of the plot can sense the regions of mean free path on the other side of the interface.

Our calculations contain any effects that arise from potential steps at the interfaces or from quantum well states. It is clear that there are discontinuities in all of the conductivities; majority, minority, and AP at the interfaces between cobalt and copper. Model calculations which we have performed using the free electron model and steps of various sizes indicate that they may have large effects on the conductivities but the effects on the GMR are usually quite small. We believe that the origin of the GMR in figure 6 is not the step but the fact that although the scattering rates are the same for all layers and spin channels, the mean free path for minority cobalt is significantly smaller than for majority cobalt.

### Interfacial Scattering

In order to evaluate the effect of strong interfacial scattering we calculated the non-local layer dependent conductivities for 10 copper (111) planes embedded in cobalt. We attempted

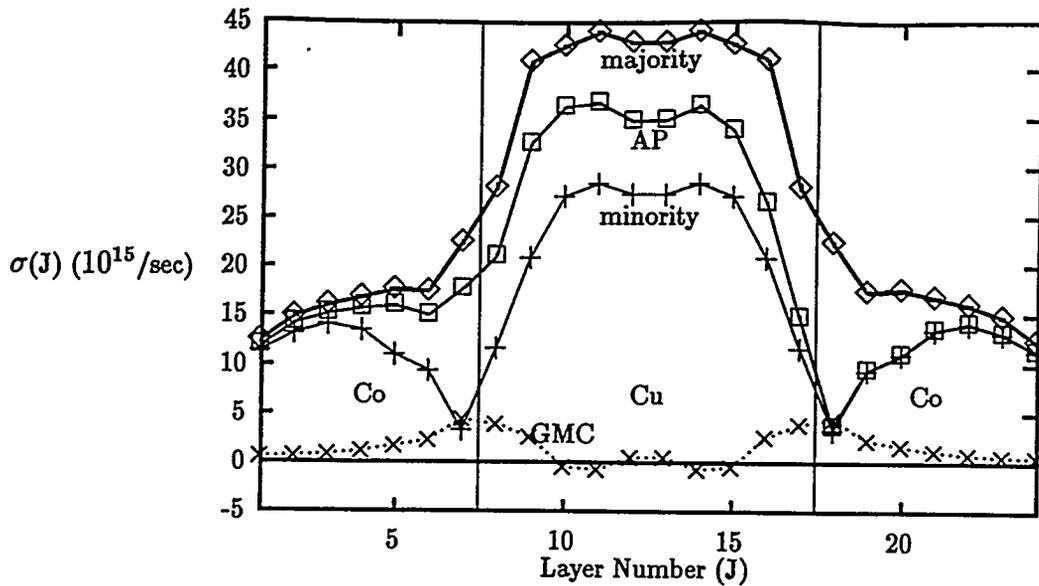


Figure 7: Layer dependent conductivities for strong interfacial scattering.

to model a system in which the copper resistivity is  $2.8 \mu\Omega \text{ cm}$  and the cobalt resistivity is  $14.8 \mu\Omega \text{ cm}$ . These values seem to be typical of sputtered films[21]. We assumed that the electron lifetimes in the majority and minority spin channels were the same in cobalt (.0025 Hartrees). This would lead to very nearly the same conductivities in the two channels for a system that is entirely cobalt. In addition we assumed that due to intermixing at the interface, the scattering rate for majority spin cobalt at the interfacial layer is twice that in the bulk and for the minority spin it is 24 times that of the bulk. This factor of 12 between the scattering rates of minority and majority spin electrons is based on coherent potential approximation calculations that we performed of the resistivity due to copper impurities in cobalt and (spin aligned) cobalt impurities in copper. The scattering rates for the copper interfacial layer were chosen to be 3.4 and 6.8 times that in bulk copper (.0006 Hartree) respectively for the majority and minority spins. The calculated GMR ( $\Delta R/R_p$ ) for the assumed geometry and scattering rates is 0.035.

Figure 7 shows the layer dependent conductivities. The effect of the interfacial scattering is to strongly depress the minority conductivity in the vicinity of the interface where the strong scattering was assumed. The GMR is seen to be greater for the case with interfacial scattering than for the case in which it was ignored.

### Bulk and Interfacial Scattering

The calculations presented in the previous section assumed that the majority and minority lifetimes are the same in the cobalt layers. The scattering rates that occur in practice will depend on the scattering mechanism. For each spin channel, the probability of a scattering event is proportional to the number of final states. For most scattering mechanisms such as nonmagnetic impurities or phonon scattering it means that the scattering rate is proportional to the density of states of the given spin channel at the Fermi energy. Because the density of states is usually much higher at the Fermi energy for the minority spin, the lifetime of minority electrons is usually much shorter than that of majority electrons. Figure

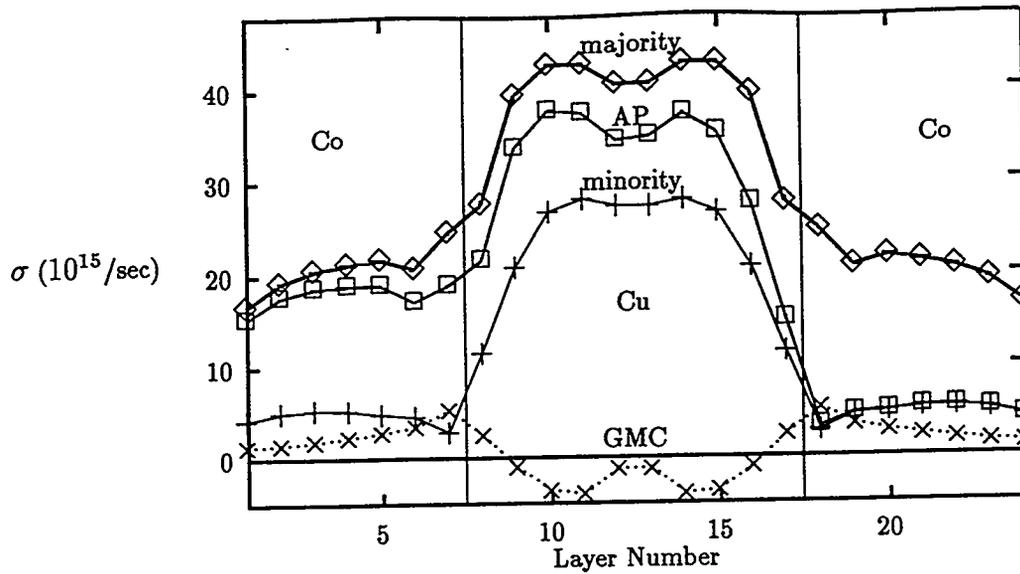


Figure 8: Layer dependent conductivity in the presence of both interfacial and bulk scattering.

8 shows the calculated layer dependent conductivity assuming that the electron lifetime for majority carriers in the cobalt layers is seven times that in the minority layers due to the difference in Fermi Energy density of states,  $\hbar/\tau = .0014, .01008$  for majority and minority, respectively. The GMR in this case is  $\Delta R/R_p = .024$ .

It is interesting that the introduction of an asymmetry in the bulk scattering rates actually decreased the GMR compared to the result of figure 7. The GMR actually increases substantially in the cobalt but this is more than offset by the decrease in the copper. The decrease in the copper can be traced to the fact that decreasing the scattering rate for the majority electrons in the cobalt *lowers* the conductivity of these electrons in the copper. The overall conductivity is however increased as expected and the GMR would probably have increased if the bulk cobalt layers had been thicker.

## Conclusions

We have shown that the Kubo formalism can be evaluated with the Layer-KKR formalism to calculate the non-local layer dependent conductivities and GMR from first principles. We have shown that GMR in the CIP geometry is an inherently non-local phenomenon and that the largest contributions to the GMR come from currents carried near one interface arising from fields sensed near the other interface. Our results also demonstrate that the effects of electronic structure and scattering rates on the conductivity and GMR can be quite subtle.

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# First Principles Calculation of Electrical Conductivity and Giant Magnetoresistance of Co|Cu Multilayers

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## ABSTRACT

We show that the Kubo formula can be used to calculate the non-local electrical conductivity of layered systems from first principles. We use the Layer Korringa Kohn Rostoker method to calculate the electronic structure and the Green function of Co|Cu|Co trilayers within the local density approximation to density functional theory. This Green function is used to calculate the conductivity through the Kubo formula for both majority and minority spins and for alignment and anti-alignment of the Co moments on either side of the Cu spacer layer. This allows us to determine the giant magnetoresistance from first principles. We investigate three possibilities for the scattering in Co|Cu|Co: (1) equal electron lifetimes for Cu, majority spin Co, and minority spin Co, (2) equal electron lifetimes for majority and minority Co, weaker scattering in Cu and spin dependent interfacial scattering, (3) electron lifetimes for majority and minority spin cobalt proportional to their Fermi energy densities of states and spin dependent interfacial scattering.

## Introduction

Recently there has been great interest in the transport properties of layered magnetic materials because of the discovery of a new form of magnetoresistance[1, 2] called the giant magnetoresistance (GMR). GMR is a change (generally a pronounced decrease) in the electrical resistance of an inhomogeneous system that is observed when an applied magnetic field causes an alignment of the magnetic moments in different parts of the material. GMR has been observed in several geometries, but the most promising and interesting GMR systems are composed of thin layers of ferromagnetic material separated by non-magnetic or very weakly magnetic spacer layers.

The transport properties of layered materials have been the subject of several theoretical investigations based on the model of free electrons with random point scatterers (FERPS). Using this model, Fuchs[3] and later Sondheimer[4] obtained a solution to the semi-classical Boltzmann equation with boundary conditions appropriate to free electrons in a thin film. Barnás and coworkers[5] extended this approach to the case in which the film has several layers with differing scattering rates. Levy and coworkers[6, 7, 8, 9, 10] applied the more rigorous Kubo-Greenwood[11, 12] formula to the FERPS model and developed two different approximations for transport in magnetic multilayers. Zhang and Butler[13] have recently evaluated the Kubo-Greenwood formula exactly for the FERPS model applied to multilayers. Their results allow a comparison of the relative success of the various approximations in representing the conductivity of the free electron model. They found that the semi-classical

approximation works surprisingly well for the FERPS model applied to multilayers.

In addition to theoretical treatments of GMR based on the FERPS model there have been a few previous applications of first principles techniques. Butler, *et. al.*[14] calculated the GMR for periodic multilayers of copper and cobalt and of copper and permalloy ( $\text{Ni}_8\text{Fe}_2$ ). They calculated the complex energy bands using the coherent potential approximation and showed that the imaginary part of the crystal momentum can be interpreted as the inverse of twice the electron mean free path. Their calculations showed that there is the potential for a very large GMR due to spin dependent interfacial scattering because the Fermi energy scattering amplitudes for majority spin cobalt, majority spin nickel and majority spin iron (as an impurity in nickel) are all very similar. Nesbet[15] reached a similar conclusion in studies of periodic  $\text{Cu}_2\text{Co}$  multilayers. Schep *et. al.*[16] have investigated a very different form of GMR from that seen experimentally by assuming that electron transport is *ballistic* rather than diffusive.

In this paper we report on first-principles calculations of the electronic structure of cobalt-copper multilayers. Using this electronic structure we calculate the conductivity by evaluating the Kubo-Greenwood linear response formula. We do not assume that the scattering is weak or that the electron wave functions are those of free electrons nor do we make the semi-classical approximations necessary to apply Boltzmann theory. It should also be noted that our approach does not require periodicity perpendicular to the layers so that it can be applied to spin valves and trilayers.

## Conductivity of Inhomogeneous Systems

We define the nonlocal conductivity  $\sigma_{\mu\nu}^s(\mathbf{r}, \mathbf{r}')$  as the linear response of the current of electrons of spin  $s$  at point  $\mathbf{r}$  in direction  $\mu$  to the local applied field at point  $\mathbf{r}'$  in direction  $\nu$ ,

$$J_{\mu}^s(\mathbf{r}) = \int d\mathbf{r}' \sum_{\nu} \sigma_{\mu\nu}^s(\mathbf{r}, \mathbf{r}') E_{\nu}^s(\mathbf{r}'). \quad (1)$$

Here "local applied field" means the change in the local electrostatic field that arises due to the application of a potential difference across the sample. For an inhomogeneous system this may differ from the average applied field and it may be different for different spins[8].

For a homogeneous system, the current and applied field can be assumed to be uniform so that one can define a single conductivity which is also uniform,  $J_{\mu}^s = \sum_{\nu} \sigma_{\mu\nu}^s E_{\nu}$ . This is the conductivity which is given by the Kubo-Greenwood formula[11, 12],

$$\sigma_{\mu\nu}^s = \frac{\pi\hbar}{N\Omega} \left\langle \sum_{\alpha, \alpha'} \langle \alpha | j_{\mu} | \alpha' \rangle \langle \alpha' | j_{\nu} | \alpha \rangle \delta(\epsilon_F - \epsilon_{\alpha}) \delta(\epsilon_F - \epsilon_{\alpha'}) \right\rangle \quad (2)$$

where  $j_{\mu}$  is the current operator,  $j_{\mu} \equiv (-i\hbar e/m_e)\partial/\partial r_{\mu}$ ,  $\Omega$  is the volume per atom and  $N$  is the number of atoms. The quantum states  $|\alpha\rangle$  in Eq. (2) represent the exact eigenfunctions of a particular configuration of the random potential, and the large angle brackets indicate an average over configurations.

In order to define a non-local site dependent conductivity,  $\sigma_{\mu\nu}^{i,j,s}$ , we define the current density at site  $i$  for spin  $s$  as the average of the current density over the atomic cell at that site,  $J_{\mu}^{i,s} = \Omega_i^{-1} \int_{\Omega_i} d\mathbf{r} J_{\mu}^s(\mathbf{r})$ . We also assume that the local field,  $E_{\nu}^s(\mathbf{r})$ , is constant over each atomic cell. Thus we write Ohm's law in a discrete form in which the current at site  $i$  is

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