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An approximate calculation for transport in magnetic tunnel junctions in the presence of localized states

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ABSTRACT

In conventional calculations of transport in magnetic tunnel junctions, one usually assumes that the transverse momentum of the tunnelling electrons is conserved and that the itinerant electron states are orthogonal to localized states. However, in most of the junctions studied, there is diffuse scattering in both the bulk of the electrodes and the barrier so that the transverse momentum is not conserved, and there are processes that couple localized states at the electrode–barrier interface to the itinerant states in the bulk of the electrodes. While it is in principle possible to include these effects, it leads to lengthy calculations. Here we propose an approximate scheme in which we do not take explicit account of either of the effects mentioned above, but in which we calculate the tunnelling through all the states that exist at the electrode–barrier interfaces. We compare the $\mathbf{k}_{\|}$-resolved density of states and tunnelling currents across a junction in our approximate scheme with that found using the Landauer formalism in the ballistic limit.

Measurements of the resistance and magnetoresistance of magnetic tunnel junctions (MTJs) are usually made by passing a current with voltage probes far removed from the interfaces between the electrodes and insulating barrier. Therefore it makes sense to calculate these transport properties as the transmission probability of going from eigenstates in one lead (electrode) to those of the other. This is the essence of the Landauer–Büttiker (LB) formalism which equates the current to the probability of transmission between sets of eigenstates in the leads (Datta 1995). While this formalism can take into account diffuse scattering in the junction most calculations are made in the purely ballistic limit; so one has conservation of momentum parallel to the planes of the layers perpendicular to the current.

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Also, the complete eigenvalue spectrum of a semi-infinite solid contains states localized at the surface as well as the continuum for the bulk (Zangwill 1988). If the energies of the surface states lie in the gaps between the bands of the bulk states, they form localized states; otherwise they are resonant states, that is, mixtures of localized surface and itinerant band states. At a surface the electronic structure, for example, the local density of states (DOS), which is a projection of the eigenvalue spectrum in a spatially local region, contains these localized and resonant states; in the bulk of a metal no weight is given to surface states in the electronic structure. In metallic multilayered structures, states localized at interfaces appear in much the same way as surface states. In tunnel junctions these states may couple to excited states in the barrier better than the itinerant states; therefore they can increase the tunnelling conductance *if* there are mechanisms for electrons arriving in itinerant states from the leads to scatter into these localized states as well as for electrons to exit from states on the other side of the barrier. If these states lie on the Fermi level and at $T = 0\,K$, these interfacial or barrier states contribute if processes exist that elastically scatter electrons from the itinerant to surface states of the metallic electrodes and vice versa; this comes from impurities and roughness of the interface or surface. When electrons tunnel across a biased junction, they undergo inelastic scattering, and surface states contribute if this takes place at the metal–barrier interface, even if they do not lie at the Fermi level. However, by calculating the electronic structure and eigenstates far from the interfaces these localized states are not considered in a purely ballistic treatment, even if they lie on the Fermi surface, since they are orthogonal to the delocalized states and therefore cannot carry a steady-state current. In principle it is possible to take account of the contribution of these localized states to tunnelling conduction; however, it is a rather difficult calculation, and one usually does not consider their contribution.

Here we suggest an approximate scheme which is to calculate the transport as if the DOS in the leads were replaced by those at the electrode–barrier interfaces. While we do not explicitly take into account the diffuse scattering in the electrodes or at the interfaces, all the states at the electrode–barrier interfaces, localized as well as itinerant, contribute to tunnelling. In this way we accent the role of the interfacial DOS in controlling tunnelling. We compare the $\mathbf{k}_{\|}$-resolved DOS and tunnelling currents for model MTJs with vacuum barriers found with our scheme with those in the traditional LB approach in which one does not take account of diffuse scattering or localized states. Comparisons with data as they become available will eventually determine whether our approximation or the ballistic LB approach is better able to represent the features of the electronic structure that control tunnelling in MTJs.

The following estimates tell us whether the scattering rates are sufficient for localized states to participate in conduction. The lifetime due to electron–electron interaction is (V. Qi 2000, private communication),

$$\frac{1}{\tau_{e-e}} \simeq \frac{1}{\mathsf{p}} \frac{\pi^2}{16 E_F} (kT)^2, \tag{1}$$

where p is Planck's constant and E_F is the Fermi energy. The tunnelling rate is estimated from the Wentzel–Kramers–Brillouin approximation as

$$\frac{1}{\tau_t} = \frac{1}{\mathsf{p}} C \exp(-2kd), \tag{2}$$

where C is of the order of 1 eV, $k \cong 1\text{Å}^{-1}$ is the decay length in the barrier and d is the thickness of barrier which we take to be between 10 and 15 Å. By comparing these two expressions, we find the relaxation rate (1) is faster than the tunnelling rate (2) when $T > 14\,\text{mK}$ for 15 Å barriers, and 2 K for 10Å barriers. Also we can estimate the role of electron–phonon interactions. For acoustic phonons the relaxation rate is given by (Mahan 1990)

$$\frac{1}{\tau_p} \sim \frac{1}{p}\frac{3}{\pi}\frac{(kT)^3}{\omega_D^2}, \tag{3}$$

where ω_D is the Debye energy in units of temperature (approximately equal to 300 K). This rate is comparable with that from electron–electron scattering at $T \approx 4\,\text{K}$. These relaxation rates are fast enough to populate localized states at the Fermi level, even for ideal structures at the lowest temperatures at which MTJs have been studied.

As real junctions have impurities and defects, the relaxation rate is actually faster than the above estimates for ideal junctions. The mean free path in a magnetic electrode is of the order of 100Å; this is equivalent to a scattering rate of the order of $1/\tau_{imp} = 10^{14}\text{s}^{-1}$. As the tunnelling rate estimated from equation (2) is only $10^6\,\text{s}^{-1}$, the relaxation rate due to the impurity scattering is usually much larger. Parenthetically, for currents perpendicular to the plane of the layers in metallic multilayered structures there is no exponential decay factor in (2); so in place of the tunnelling rate we have a rate that is of the order of $10^{15}\,\text{s}^{-1}$. Thus, it is reasonable to calculate the conductance in metallic multilayers by neglecting the relaxation mechanisms mentioned here.

We have calculated the conductance of transition-metal–vacuum tunnel junctions by using the Caroli (1971, 1972) formalism (Combescot 1971, Todorov *et al*, 1993). While real junctions have insulating barriers we have taken a vacuum as it is the simplest insulator for which we can make an *ab-initio* calculation. In the linear response region, the conductance for a finite conductor is (Wang 1999, Wang *et al.* 2001)

$$G = \frac{2\pi e^2}{p}\text{Tr}\Bigg(\int d\mathbf{k}_\parallel \{\rho^\alpha(\mathbf{k}_{\parallel,\epsilon_F})[t^\dagger(\mathbf{k}_{\parallel,\epsilon_F})]^{\alpha\beta} \times \rho^\beta(\mathbf{k}_{\parallel,\epsilon_F})t(\mathbf{k}_{\parallel,\epsilon_F})^{\beta\alpha}\}\Bigg), \tag{4}$$

where $t^{\alpha\beta}$ is the **t**-matrix between α and β, the bounding surfaces across which the current is coherent which in our case will be the electrode–barrier interfaces; the trace Tr is over all (site and angular momentum, or energy level) indices; the DOSs ρ^α and ρ^β at the Fermi level used in this formalism are those at a surface created by cutting the junction so that the two parts thereby created are isolated from one another (Pollman and Pantelides 1978).

To calculate the **t**-matrix, we first determine the propagator **G** from a full junction calculation and then backward derive $t^{\alpha\beta}$ from the Dyson equation $\mathbf{G} = \mathbf{g} + \mathbf{gVG} = \mathbf{g} + \mathbf{gtg}$, where **g** is the propagator in the absence of the perturbation **V**. In our case, **V** joins the electrodes on each side of a vacuum barrier of six monolayers; it represents the coupling of the conductor to the leads (Datta 1995, Wang 1999, Wang *et al.* 2001). We adopted an empty lattice that contains no atoms for the vacuum layers. By definition $g^{\alpha\beta}$ is zero and **V** is reasonably well localized so

that we make the approximation of considering it as a nearest-neighbour interaction (in a description in which we use two atomic layers per principal layer so that we have indeed nearest- and next-nearest neighbour interactions (Szunyogh *et al.* 1994)); we find that

$$G^{\alpha\beta} \approx g^{\alpha\alpha} t^{\alpha\beta} g^{\beta\beta}. \tag{5}$$

Upon inversion this yields the **t** matrix; $t^{\alpha\beta}$ across the barrier is quite different from those for α and β taken deep in the electrodes; this is reasonable inasmuch as the physical conductors in these two cases are different. By inserting this result in (4) to calculate the conductance, we are treating the transport between α and β coherently inasmuch as we explicitly use the propagator $G^{\alpha\beta}$ and, because we do not keep track of the momentum outside α and β, the transport in the electrodes is treated as if it was diffusive. This interpretation comes from the derivation of equation (1) (for example see Datta (1995)).

To compare the conductances obtained in this approach with calculations in which transport is considered coherent across the entire junction we calculated the conductance for bcc Fe(100)/vacuum/Fe, and for fcc Co(100)/vacuum/Co tunnel junctions from band structures obtained from the spin-polarized scalar-relativistic screened Korringa–Kohn–Rostoker method (Szunyogh *et al.* 1994). The atomic-sphere approximation (ASA) is used; while this is an approximation it does not alter the main point that we are making about the two different approaches to calculating the conductance of a MTJ. Here we present the results for Fe; they are further corroborated by those on Co. The lattice parameter for Fe is 5.27 au. Two atomic layers are included in each screened principal layer, and the screening potential is set to 2 Ry inside each atomic cell. The Gunnarsson–Lundqvist (1976) exchange-correlation potential is used, and energy integration is performed by means of Gaussian quadrature with 16 points on a semicircle in the upper half complex energy plane. For self-consistent calculations of the bulk metal, the free metal surface and the metal–vacuum–metal interface potentials, 45 $\mathbf{k}_\parallel$ points are used in the irreducible wedge of the two-dimensional Brillouin zone, which enables the Fermi level to be converged up to 10^{-7} Ry. For more details of this method see Szunyogh *et al.* (1994). We used a small imaginary part of the energy of $\epsilon = 0.5$ mRy in the propagators in order to converge our results in a reasonable time. As this has a different effect on the states in the electrodes (metallic conduction) and the evanescent states in the barriers, we shall not dwell on differences in the absolute values of the conductances we calculate for finite ϵ directly across and far from the barrier. Rather we stress the qualitative differences, for example symmetries, in the $\mathbf{k}_\parallel$-resolved conductances in the two cases.

In figures1 (*a*) and (*b*) we show the $\mathbf{k}_\parallel$-resolved surface and bulk DOS for the minority channel for Fe/vacuum/Fe junctions at $\epsilon = \epsilon_F - 0.05$ eV. As we indicate below, this energy corresponds to the position of a localized state; therefore the DOS includes a strong peak about $\mathbf{k}_\parallel = \mathbf{0}$ which is not there at ϵ_F. In figures 1 (*c*) and (*d*) we show conductances calculated across the barrier and far from it, for Fe/vacuum (4 monolayers)/Fe all at the Fermi level. We note the strong correlation between the surface DOS (without the peak at $\mathbf{k}_\parallel = \mathbf{0}$) and conductance calculated directly across the barrier.

Let us turn our attention to the putative contribution of states localized at the electrode–barrier to tunnelling. In ferromagnetic metals such as Fe(100) the existence of localized states at the surface has been known for some time (Gadzuk 1979,

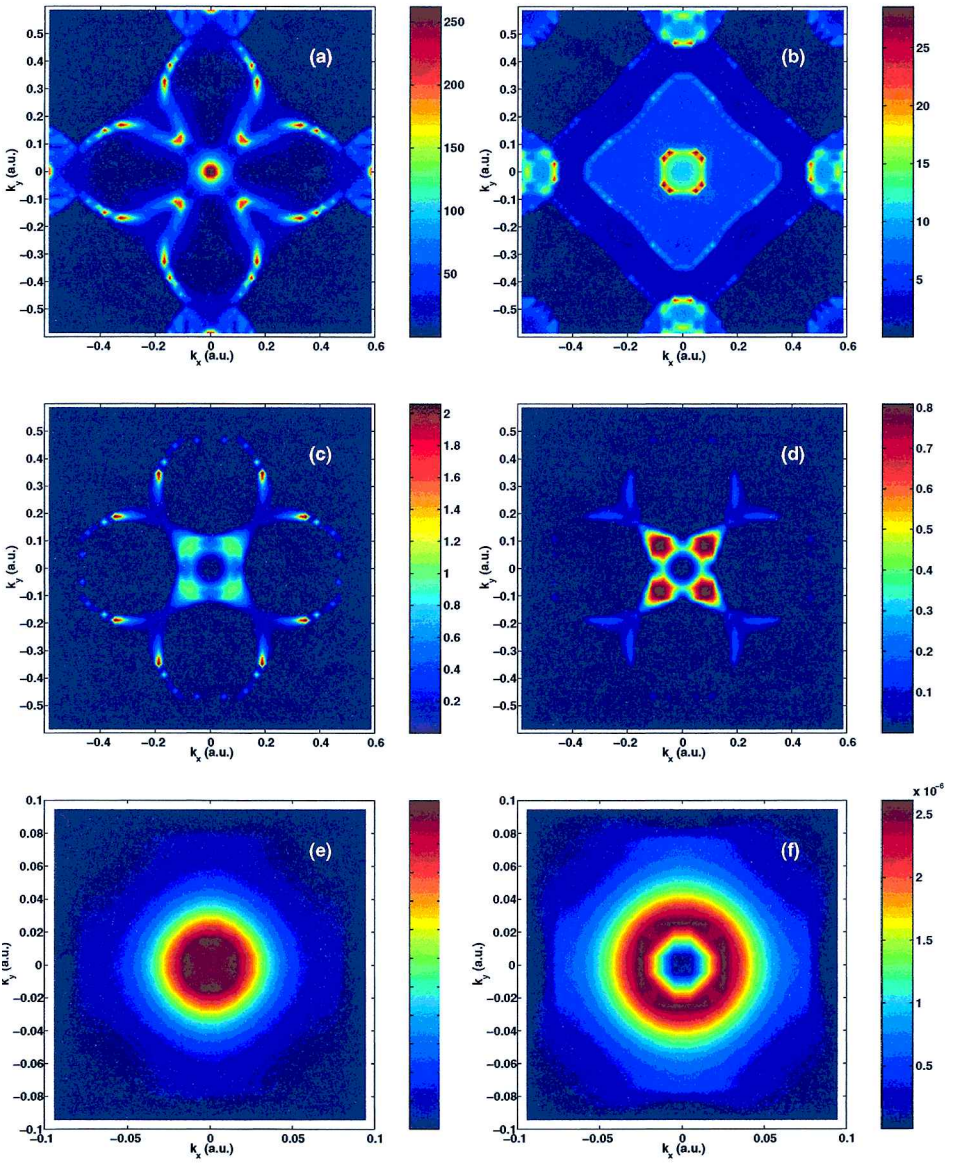

Figure 1. $\mathbf{k}_{\|}$-resolved plots in the minority channel. The DOS of the Fe electrodes is shown for $E_F - 0.05\,eV$ (*a*) at the surface (note the high density around $\mathbf{k}_{\|} = \mathbf{0}$ which is due to a localized state that would be absent at E_F) and (*b*) in the bulk (which is more or less the same at E_F). The conductances of a Fe/vacuum (4 monolayers)/Fe barrier are presented at E_F (*c*) directly across the interfaces and (*d*) seven layers from the barrier. A similar conductance plot is given for Fe/vacuum (10 monolayers)/Fe at $E_F - 0.05\,eV$ where we can focus on the centre of the zone (*e*) directly across the interfaces and (*f*) seven layers away.

Stroscio *et al.* 1995); more recently, surface states were also observed in Gd(0001) (Bode *et al.* 1998, 1999). If the energies of the surface states lie in the gaps between the bands of the bulk states, they form true localized states; otherwise they are resonant states, that is admixtures of itinerant and localized states. When one treats

the entire junction coherently, tunnelling is certainly affected by these resonant states at the interfaces of the junction; see for example figure 2(*b*) in the paper by MacLaren *et al.* (1999) where these resonances appear along the Γ–M direction away from the zone centre. However, the true localized states, on the contrary, are orthogonal to resonant and itinerant states; therefore coherent transport will be unaffected by them. Nonetheless, it has been shown that the conductance through the localized states at Fe–vacuum and Gd–vacuum interfaces can be substantial because these states have orbits that point out from the surface into the barrier (Gadzuk 1979, Stroscio *et al.* 1995, Bode *et al.* 1998, 1999). This further emphasizes the diffusive nature of the transport in the electrodes and the ambient relaxation that allows the localized states to contribute to conduction; both of these are neglected in the approach where we assume coherent, that is ballistic, transport for the entire junction.

At the Fe(100)–vacuum interface, surface states exist in the minority channel at the Fermi level for $\mathbf{k}_{\|} \neq \mathbf{0}$; for $\mathbf{k}_{\|} \approx \mathbf{0}$ localized states exist above ϵ_{F} (Gadzuk 1979, Stroscio *et al.* 1995, Bode *et al.* 1998, 1999, Papanikolaou *et al.* 2000); therefore those with $\mathbf{k}_{\|} \approx \mathbf{0}$ contribute to tunnelling if one applies a bias. In our ASA calculations there are only surface resonant states at ϵ_{F}, and we have found localized states in the minority channel about $\mathbf{k}_{\|} \approx \mathbf{0}$ just below the Fermi level at $\epsilon \approx \epsilon_{\mathrm{F}} - 0.05\,\mathrm{eV}$. In figures 1(*e*) and (*f*) we show the conductance 0.05 eV below the Fermi level calculated across the barrier and deep in the electrodes; we use 10 monolayers of vacuum to demonstrate the role of the localized state in promoting transport about $\mathbf{k}_{\|} \approx \mathbf{0}$. The large DOS at the surface about $\mathbf{k}_{\|} = \mathbf{0}$ at 0.05 eV below the Fermi level, which is absent at ϵ_{F} as well as in the bulk DOS at $\epsilon = \epsilon_{\mathrm{F}} - 0.05\,\mathrm{eV}$ (not shown) indicates the presence of a localized surface state. On comparing these conductances with those in figures 1(*c*) and (*d*) (this time for 10 monolayers of vacuum), only the conductance for the barrier and at $\epsilon_{\mathrm{F}} - 0.05\,\mathrm{eV}$ has a strong contribution from the localized states about $\mathbf{k}_{\|} = \mathbf{0}$; all the other conductances have no contributions about $\mathbf{k}_{\|} = \mathbf{0}$. One notes that the average of the conductance calculated across the barrier at $\epsilon_{\mathrm{F}} - 0.05\,\mathrm{eV}$ is four times than at ϵ_{F}.

The conclusion that can be drawn is that one cannot have truly localized states contributing to the tunnelling conduction when one treats the entire junction coherently, which one does in a LB approach with $\mathbf{k}_{\|}$ conserved. The assumption of coherent conduction across an entire junction overestimates the effect on tunnelling of the matching of states in the bulk of the electrodes to those at the interface and, if they are present, overlooks contributions from states localized near the interfaces that are coupled to itinerant states in the electrodes by diffusive and relaxation processes in real planar junctions. In our approximate scheme any state that exists at the electrode–barrier interface will be populated by the leads. It remains to be seen whether, in real junctions, localized states are mixed with resonant and itinerant states at the interfaces so that they contribute to the conduction as measured across electrodes far from the barrier.

We have used a vacuum whereas the barriers in the tunnel junctions studied to date have been insulators; while this changes the conductance that one calculates, it does not alter the conclusion that we arrive at. For a finite bias, one probes a larger region about the Fermi level so that localized surface states away from ϵ_{F} contribute to conduction; their contribution to the conductance will be included if one does the

calculation directly across the barrier rather than in the electrodes far from the barrier.

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