Eur. Phys. J. B **10**, 599–606 (1999)

THE EUROPEAN PHYSICAL JOURNAL B

EDP Sciences

Models for magnetoresistance in tunnel junctions

S. Zhang[1] and P.M. Levy[2,a]

[1] Department of Physics, University of Missouri-Rolla, Rolla, MO 65409, USA
[2] Department of Physics, New York University, 4 Washington Place, New York, NY 10003, USA

Received 9 January 1999 and Received in final form 10 February 1999

Abstract. We show there are putative pitfalls when one predicts the magnetoresistance of magnetic tunnel junctions (JMR) based on different toy models. Amongst them are the sensitivity of the MR to the details of the profile of the potential barrier between the metallic electrodes and the insulating barrier, and the common assumption of only one band of electrons. We indicate the ingredients that are necessary to obtain a more complete description of the JMR of magnetic tunnel junctions.

PACS. 73.40.Gk Tunneling – 73.50.Jt Galvanomagnetic and other magnetotransport effects (including thermomagnetic effects) – 75.70.Cn Interfacial magnetic properties (multilayers, magnetic quantum wells, superlattices, magnetic heterostructures)

1 Introduction

The recent success in growing magnetic tunnel junctions (MTJ's) [1,2] has lead to a resurgence of interest in their magnetoresistance (JMR). As tunnel junctions have been studied over the past four decades a number of toy models (theoretical approaches with simplifying assumption) have been used to understand experimental data; one can classify these approaches into two broad categories: continuous [3] and lattice [4] models. Within a continuous model, the existence of lattice sites is overlooked and the electronic structure for the electrodes are assumed to be those of the metal in bulk form, *i.e.*, one overlooks the variation of the band structure in a metallic electrode near its interface with the insulating barrier. In this approach, by suitably choosing a model potential for the insulating barrier, transmission coefficients for electrons from left to right electrodes can be calculated and thereby the conductance and tunnel current. While the calculations can be done exactly for a given electronic structure and potential profile of the barrier, it is hard to justify these model potentials. We will show that magnetoconductance depends strongly on the profile of the barrier potential, therefore approximations for the barrier potential can introduce severe errors in predicting conductance and magnetoresistance of a tunnel junction (JMR). In lattice models, one distinguishes electronic structures at interfaces from that in the bulk. As it is not possible to do self consistent equilibrium calculations in the presence of a finite potential across a junction one breaks it up into isolated systems so that they are non-conducting. Then one uses the Keldysh formalism [4] to derive conductance when interactions between these isolated systems are turned on.

Here we wish to clarify some of the ambiguous conclusions and contradictory results derived from these two approaches. The paper is organized as follows. In Section 2, we consider a free electron one band (continuous) description of tunneling through a barrier and demonstrate that the conductance is sensitive to the details of the barrier potential. Next we review the transfer Hamiltonian method and point out the importance of considering the contributions from several bands to tunneling in order to avoid the cancellation of the density of states in the tunneling current. In Section 4, a tight-binding lattice description is discussed, and in Section 5 the effects of interfacial roughness on tunneling are taken into account. We summarize the strengths and deficiencies of the approaches we have outlined in the concluding section.

2 Free electron models

Let us consider free electrons in a MTJ consisting of metal(1)/insulator/metal(2). The flat potentials of metal(i) ($i = 1, 2$) are V_i, and the barrier potential is $U(x)$. If the metallic electrodes are magnetic, the potentials V_i have spin indices. Since we do not consider spin-flip processes each spin channel can be treated independently; therefore we drop the spin labels and show them only when they are needed. The junction possesses translation invariance in the plane of the layers that comprise the junction, therefore momentum parallel to the planes ($\mathbf{k}_{||}$) is conserved. The wavefunction of an incoming wave

[a] e-mail: levy@nyu.edu

from the left electrode (1) is

$$\Psi(\mathbf{r}) = \phi_1(x)\exp(\mathrm{i}k_\parallel \cdot r_\parallel) \tag{1}$$

where

$$\phi_1(x) = \exp(\mathrm{i}k_1 x) + r\exp(-\mathrm{i}k_1 x),$$

for $x < 0$,

$$\phi_2(x) = t\exp(\mathrm{i}k_2 x),$$

for $x > d$, and the wave function in the barrier region satisfies the equation

$$\frac{\hbar^2}{2m}\phi_{\mathrm{b}}''(x) = \left(\epsilon - \frac{\hbar^2 k_\parallel^2}{2m} - U(x)\right)\phi_{\mathrm{b}}(x),$$

for $0 < x < d$. Here d is the thickness of the barrier, and $k_{1,2} = \sqrt{2m(\epsilon_{\mathrm{F}} - V_{1,2})/\hbar^2 - \mathbf{k}_\parallel^2}$. For a given potential profile, one can determine the wavefunction in the barrier, and the transmission amplitude t can be found by matching wavefunctions and their derivatives at $x = 0$ and $x = d$. If one chooses a square potential barrier, Slonczewski found the conductance is [3]

$$G = (e^2/\hbar)\sum_{k_\parallel,\sigma}\frac{16k_1k_2k_{\mathrm{b}}^2\exp(-2k_{\mathrm{b}}d)}{(k_1^2+k_{\mathrm{b}}^2)(k_2^2+k_{\mathrm{b}}^2)} \tag{2}$$

where $k_{\mathrm{b}} = \sqrt{2m(U-\epsilon_{\mathrm{F}})/\hbar^2 + k_\parallel^2}$. From this one might conclude that in the limit of a high barrier potential ($k_{\mathrm{b}} \gg k_1\, k_2$) the tunnel conductance is proportional to the density of states of the electrodes (k_1 and k_2).

Unfortunately, such a conclusion is limited to this special choice of the square potential, *i.e.*, where the potential changes abruptly. To see this, let us assume the potential varies rather slowly so that the WKB approximation is valid. Then the wavefunction is given by,

$$\phi(k_\parallel, x) = \frac{C}{\sqrt{k_x(x)}}\exp\left(\mathrm{i}\int^x k_x(x_1)\mathrm{d}x_1\right) \tag{3}$$

where C is the normalization constant. From the definition of the transmission amplitude, below equation (1), we have

$$t = \frac{\phi(k_{||}, d)}{\phi(k_{||}, 0)} = \sqrt{\frac{k_1}{k_2}}\exp\left(-\int_0^d k_{\mathrm{b}}(x)\mathrm{d}x\right)$$

where we have defined $k_{\mathrm{b}}(x) = \mathrm{i}k_x(x)$ to represent the imaginary momentum in the barrier. By using this transmission amplitude, the WKB conductance is,

$$\begin{aligned} G &= (e^2/\hbar)\sum_{\mathbf{k}_{||},\sigma}|t|^2 k_2/k_1 \\ &= (e^2/\hbar)\sum_{\mathbf{k}_{||},\sigma}\exp\left(-2\int_0^d k_{\mathrm{b}}(x)\mathrm{d}x\right). \end{aligned} \tag{4}$$

By comparing equations (2, 4), one clearly sees that the density of the state factor does *not* enter the tunnel conductance in the WKB approximation. As the actual potential in a junction changes on the scale of a lattice constant, neither the abrupt change nor the slow variation in the barrier potential are realistic for modeling actual tunnel junctions. We conclude that tunnel conductance is quite sensitive to the details of potential profiles.

To make this more apparent we choose a square potential barrier (as for Eq. (2)) with an extra step at both sides of the interface, *e.g.*, the potential is given by U' for $0 < x < a_0$ and $d - a_0 < x < d$ and U for $a_0 < x < d - a_0$, where a_0 is the width of the step at either side of the interface. In this case, a tedious yet straightforward calculation lead to the conductance

$$G = (e^2/\hbar)\sum_{\mathbf{k}_{||},\sigma}\frac{16k_1k_2k_{\mathrm{b}}^2\exp(-2k_{\mathrm{b}}(d-2a_0))}{X_1X_2} \tag{5}$$

where

$$\begin{aligned} X_i = {} & (k_{\mathrm{b}}^2 + k_i^2)\cosh^2(k'a_0) + (k'^2 + k_{\mathrm{b}}^2k_i^2/k'^2)\sinh^2(k'a_0) \\ & - (k_{\mathrm{b}}k_i^2/k' + k_{\mathrm{b}}k')\sinh(2k'a_0), \end{aligned} \tag{6}$$

$i = 1,\ 2,\ k' \equiv \sqrt{2m(U'-\epsilon_{\mathrm{F}})/\hbar^2 + k_{||}^2}$, and we have neglected the term proportional to $\exp(-6k_{\mathrm{b}}d)$ which is much smaller than $\exp(-2k_{\mathrm{b}}d)$ since $k_{\mathrm{b}}d \gg 1$ for a typical junction. This conductance is different from that for the simple square barrier, equation (2), and the WKB result, equation (4). As $k'a_0$ is the order of one, it is hard to see from equation (6) how the conductance is related to the density of states. In Figure 1, we show the dependence of the magnetoresistance on the height of the step U', for two widths $a_0 = 0$ (abrupt potential) and 2 Å; for simplicity we have taken the high barrier limit so that only $k_\parallel = 0$ contributes to conduction in the free electron model. As the height of the step increases, the magnetoresistance first decreases to zero, the WKB result, and then increases to that of the abrupt potential. Therefore, even for the simple profiles of the potentials we have considered, magnetoresistance is quite sensitive to details of the structure of the potential barrier.

To obtain a more transparent expression for the role of the interface potential we can also include scattering at the metal-insulator interfaces. As one has frequently done for modeling the interface between a superconductor and a non-superconducting metal, we replace the extra step in the above paragraph by one with zero thickness yet with an integrated scattering strength, *i.e.*, a delta function [5]. By modeling the scattering at the metal-insulator interfaces with $U_1 = \xi_1\delta(x)$, and $U_2 = \xi_2\delta(x-d)$, the conductance equation (2) becomes

$$G = (e^2/\hbar)\sum_{\mathbf{k}_\parallel,\sigma}\frac{16k_1k_2k_{\mathrm{b}}^2\exp(-2k_{\mathrm{b}}d)}{[k_1^2 + (\xi_1 - k_{\mathrm{b}})^2][(k_2^2 + (\xi_2 - k_{\mathrm{b}})^2]}\cdot \tag{7}$$

In comparison with junctions without scattering at interfaces ($\xi_1 = \xi_2 = 0$) a significant change occurs

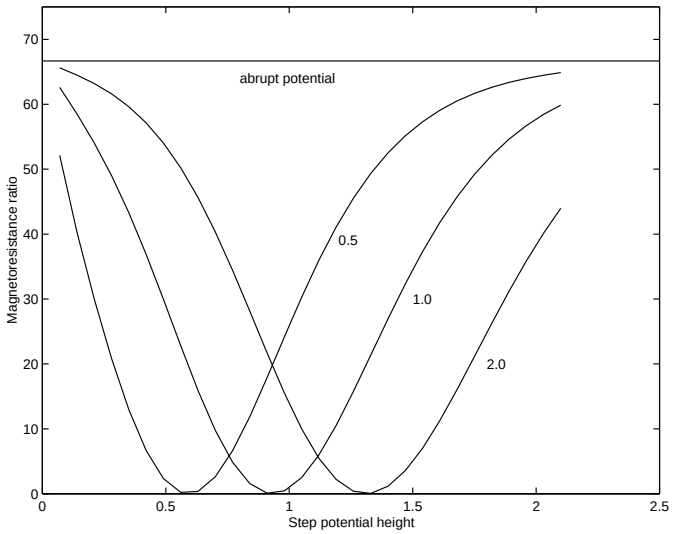

Fig. 1. The magnetoresistance ratio of a tunnel junction as a function of U', the potential of the extra steps at interfaces of the barrier and the electrodes, in the limit of a high barrier ($k_\mathrm{b} \gg k_i$). We have chosen the step width $a_0 = 2$ Å, and $k_\uparrow/k_\downarrow = 3$ for all the curves so that the magnetoresistance is 66.7% for an abrupt potential ($a_0 = 0$). The three curves are for $k_\downarrow = 0.5$ Å^{-1}, 1.0 Å^{-1} and 2.0 Å^{-1} respectively. Note that zero magnetoresistance corresponds to the WKB limit.

in the denominator of the tunnel conductance. If the scattering at the two interfaces is different, *e.g.*, $\xi_1 = k_\mathrm{b}$ (strong scattering at $x = 0$ interface) and $\xi_2 = 0$ (weak scattering at $x = d$ interface) which corresponds to a rough and a smooth interface, the conductance goes as $G \propto k_2/k_1$, *i.e.*, it is *inversely* proportional to the density of the states of one electrode and proportional to the density of states of the other. In this case, one would expect an *inverse* JMR, *i.e.*, conductance is larger when the magnetization of the electrodes are aligned antiparallel. This might explain the inverse JMR observed in junctions where the barrier is TiO/Al_2O_3 [6], and the effect seen by Moodera when a non magnetic metallic layer is inserted between the insulator and magnetic electrode [7].

Summarizing this section, we have shown that while free electron one-band models of MTJ's capture some essential features, *e.g.*, the conductance is mainly governed by the exponent of the product $k_\mathrm{b}d$, their predictions for the magnetoresistance are unreliable, because the MR is sensitive to the profile of the metal-insulator barrier potential, which is poorly known. Thus, the JMR calculated by assuming a certain profile have no quantitative significance. This dependence of tunneling in MTJ's on details of the potential comes from the size, 1-2 Å, of the wavelength of the carriers in MTJ's being comparable to the distance over which the potential changes across the metal-insulator interface. For semiconductor heterostructures, where the wavelength of the carriers is of the order of 100 Å, this problem does not appear, and it is quite acceptable to model the change in the potential between two semiconductors with an abrupt step. As we have shown elsewhere [8] the short wavelength, or inversely the large wavevector of the carriers, in MTJ's is also the cause for a loss of coherence in transmission through metallic junctions.

3 Transfer Hamiltonian

Transition metal electrodes have several bands crossing the Fermi level, therefore the question arises: which band makes the dominant contribution to tunneling? Conventional wisdom has it that the d electrons, which are spin polarized, do not contribute much to tunneling as they are tightly bound; rather its the itinerant $s-p$ electrons, which are weakly spin polarized through $s-d$ hybridization, that tunnel. From tunneling experiments into superconductors it has been established that tunnel currents are majority spin polarized for Ni, Co, Fe and their alloys [9]. This is at odds with the density of states in these metals which are larger for minority than for majority spins, *i.e.*, at least for Co and Ni. Here we show that the transfer Hamiltonian approach [10] together with the WKB approximation, which had been developed to understand superconducting junctions, is a useful way to describe tunneling when several bands are present. Among other things we show that the cancellation of the density of states in the tunneling current, and concomitantly null JMR, comes from considering only one band; when there is more than one band of electrons in the metallic electrodes there is a JMR in the WKB approximation.

The Hamiltonian for the magnetic electrodes can be written as,

$$H^p = \sum_{\mathbf{k}\sigma} \epsilon^p_{\mathbf{k}} c^p_{\mathbf{k}\sigma} c^{p+}_{\mathbf{k}\sigma} + \sum_{\mathbf{k}\sigma} f^p_{\mathbf{k}\sigma} d^p_{\mathbf{k}\sigma} d^{p+}_{\mathbf{k}\sigma} + \sum_{\mathbf{k}\sigma} W^p_{\mathbf{k}} c^{p+}_{\mathbf{k}\sigma} d^p_{\mathbf{k}\sigma} \tag{8}$$

where p represent the left ($p = \mathrm{L}$) and right ($p = \mathrm{R}$) electrodes, $c_{\mathbf{k}\sigma}$ and $d_{\mathbf{k}\sigma}$ are the annihilation operators for the itinerant (which we nominally call s although p electrons are also present) and d electrons, and $W_{\mathbf{k}}$ represents the s-d hybridization through which the itinerant (s) electrons are polarized. The Hamiltonian for the whole MTJ is,

$$H = H^\mathrm{L} + H^\mathrm{R} + H^\mathrm{T} \tag{9}$$

where H^T describes the transfer of electrons from the left to right electrodes

$$H^\mathrm{T} = \sum_{\mathbf{kq}\sigma} \Big\{ [T^{(\mathrm{c})}_{\mathbf{kq}} c^{\mathrm{L}+}_{\mathbf{k}\sigma} c^{\mathrm{R}}_{\mathbf{q}\sigma} + T^{(\mathrm{c})}_{\mathbf{qk}} c^{\mathrm{R}+}_{\mathbf{q}\sigma} c^{\mathrm{L}}_{\mathbf{k}\sigma}] + [T^{(\mathrm{d})}_{\mathbf{kq}} d^{\mathrm{L}+}_{\mathbf{k}\sigma} d^{\mathrm{R}}_{\mathbf{q}\sigma} + T^{(\mathrm{d})}_{\mathbf{qk}} d^{\mathrm{R}+}_{\mathbf{q}\sigma} d^{\mathrm{L}}_{\mathbf{k}\sigma}] \Big\} \tag{10}$$

where the $T^{(\mathrm{c,d})}_{\mathbf{kq}}$ are matrix elements describing the transfer; while they can be calculated from first principles [11] here we consider them as phenomenological parameters. JMR is sensitive to details of the potential profiles, as we showed in the preceding section, and to the coupling between electrodes and insulating barrier. The strength

of the transfer Hamiltonian approach is that one need not specify these details. For a one band description there is only one matrix element $T_{\mathbf{kq}}$ of H^{T}; in the WKB approximation it is given as [12] $T^2_{\mathbf{kq}} \propto [\rho^{\mathrm{L}}(E_{\mathbf{k}})\rho^{\mathrm{R}}(E_{\mathbf{q}})]^{-1}$ where the $\rho^{p\prime}s$ are density of states of the electrodes. As we show below the tunnel conductance is proportional to $T^2\rho^{\mathrm{L}}\rho^{\mathrm{R}}$; therefore, for a normal metal the tunnel conductance is independent of the density of states of the electrodes due to their cancellation in this product.

When there is more than one band that crosses the Fermi level one needs to specify which band(s) participate in tunneling. *We make the critical assumption that the itinerant, nominally s, electrons are the dominant electrons that participate in the tunneling.* This is clearly an ansatz, which is motivated by the form of the transfer Hamiltonian used for superconducting junctions [13,14],

$$H^{\mathrm{T}}_{\mathrm{super}} = \sum_{\mathbf{kq}\sigma}[T_{\mathbf{kq}}a^{+}_{\mathbf{k}}a_{\mathbf{q}} + \mathrm{h.c.}] \tag{11}$$

where $a_{\mathbf{k}}$ is the annihilation operator of the *normal* electron. This is equivalent to saying that only normal electrons, and not the superconductor quasi-particles, tunnel through a barrier; this was justified by noting that the presence of the barrier breaks the pairing of the superconducting electrons in the barrier. With this ansatz, Cohen *et al.* [13] were able to show that the tunnel current in a superconducting tunnel junctions is proportional to the density of the states of the superconductor. In the same spirit, we argue that $s-d$ hybridization is not present in the barrier region and only the itinerant parts (nominally s electrons) of the hybridized bands in the electrodes participate in the tunneling [15]. In analogy with superconductor junctions we suppress tunneling by d electrons in equation (10) and write the transfer Hamiltonian as,

$$H^{\mathrm{T}} = \sum_{\mathbf{kq}\sigma}[T_{\mathbf{kq}}c^{\mathrm{L}+}_{\mathbf{k}\sigma}c^{\mathrm{R}}_{\mathbf{q}\sigma} + T_{\mathbf{qk}}c^{\mathrm{R}+}_{\mathbf{q}\sigma}c^{\mathrm{L}}_{\mathbf{k}\sigma}] \tag{12}$$

where the matrix element $T_{\mathbf{kq}}$ is inversely proportional to the density of states of the electrodes, *i.e.*,

$$T^2_{\mathbf{kq}} = \frac{C^2}{\rho_{\mathrm{L}}(E_{\mathbf{k}})\rho_{\mathrm{R}}(E_{\mathbf{q}})}, \tag{13}$$

in the WKB approximation. We now show how the tunnel current can be calculated rather straightforwardly with this Hamiltonian.

The rate of change of the number of electrons in the left electrode is

$$\mathrm{i}\hbar\frac{\mathrm{d}N^{\mathrm{L}}}{\mathrm{d}t} = [N^{\mathrm{L}}, H] = [N^{\mathrm{L}}, H^{\mathrm{T}}] \tag{14}$$

where $N^{\mathrm{L}} = \sum_{\mathbf{k}\sigma}\{c^{\mathrm{L}+}_{\mathbf{k}\sigma}c^{\mathrm{L}}_{\mathbf{q}\sigma} + d^{\mathrm{L}+}_{\mathbf{k}\sigma}d^{\mathrm{L}}_{\mathbf{q}\sigma}\}$, and clearly $[N^{\mathrm{L}}, H^{\mathrm{p}}] = 0$. Explicitly, one finds

$$\mathrm{i}\hbar\frac{\mathrm{d}N^{\mathrm{L}}}{\mathrm{d}t} = \sum_{\mathbf{kq}\sigma}T_{\mathbf{kq}}[c^{\mathrm{L}+}_{\mathbf{k}\sigma}c^{\mathrm{R}}_{\mathbf{q}\sigma} - \mathrm{h.c.}]. \tag{15}$$

The tunnel current is just the average of $e\frac{\mathrm{d}N^{\mathrm{L}}}{\mathrm{d}t}$. The average $\langle c^{\mathrm{L}+}_{\mathbf{k}\sigma}c^{\mathrm{R}}_{\mathbf{q}\sigma}\rangle$ can be directly calculated by an exact equation of motion method [16] and we find

$$I = e\sum_{\mathbf{kq}\sigma}\int \mathrm{d}\epsilon|T_{\mathbf{kq}\sigma}|^2 A_{\mathrm{R}}(\mathbf{q}\sigma,\epsilon)A_{\mathrm{L}}(\mathbf{k}\sigma,\epsilon+eV) \times [n_{\mathrm{F}}(\epsilon) - n_{\mathrm{F}}(\epsilon+eV)] \tag{16}$$

where the A's are spectral functions of the s electrons, $n_{\mathrm{F}}(\epsilon)$ is the Fermi distribution function, and the transfer matrix is, according to the WKB approximation [12] inversely proportional to the product of the density of the states as given by equation (13). It remains to calculate the spectral function of s electrons. The Green's function is

$$G^p_{ss}(\epsilon) = \left[\epsilon - \epsilon^p_{\mathbf{k}} - \frac{(W^p_{\mathbf{k}})^2}{\epsilon - f^p_{\mathbf{k}\sigma}}\right]^{-1} \tag{17}$$

with poles at $\epsilon = E^p_{\mathbf{k}\sigma}$,

$$E^p_{\mathbf{k}\sigma} = \frac{\epsilon^p_{\mathbf{k}} + f^p_{\mathbf{k}\sigma}}{2} \pm \sqrt{(W^p_{\mathbf{k}})^2 + \left(\frac{\epsilon^p_{\mathbf{k}} - f^p_{\mathbf{k}\sigma}}{2}\right)^2}, \tag{18}$$

where $\epsilon^p_{\mathbf{k}}$ and $f^p_{\mathbf{k}\sigma}$ are energies of the s and d electrons; see equation (8). The residues (renormalization) at these poles are

$$Z^p_{\mathbf{k}\sigma} = \left(1 + \frac{(W^p_{\mathbf{k}})^2}{(E^p_{\mathbf{k}\sigma} - f^p_{\mathbf{k}\sigma})^2}\right)^{-1}. \tag{19}$$

Then the s electron spectral function is

$$A^p(\mathbf{k}\sigma,\epsilon) \equiv -\mathrm{Im}\ G^p_{ss} = 2\pi Z^p_{\mathbf{k}\sigma}\delta(\epsilon - E^p_{\mathbf{k}\sigma}). \tag{20}$$

By placing equations (13, 20) into equation (16), and by making a change in variables for the sum entering equation (16)

$$\sum_{\mathbf{kq}} = \int \rho_{\mathrm{L}}(E_{\mathbf{k}\sigma})\rho_{\mathrm{R}}(E_{\mathbf{q}\sigma})\mathrm{d}E_{\mathbf{k}\sigma}\mathrm{d}E_{\mathbf{q}\sigma}, \tag{21}$$

we finally arrive at

$$I = \sum_{\sigma} 2\pi e^2 C^2 \bar{Z}^{\sigma}_{\mathrm{L}}\bar{Z}^{\sigma}_{\mathrm{R}}V \tag{22}$$

where $\bar{Z}^{\sigma}$ is the average of the renormalization factor equation (19); note we have limited ourselves to low temperature and bias. While the density of states in the transfer matrix elements equation (13) cancel those in equation (21) the renormalization $\bar{Z}^{\sigma}$ contains information about the spin polarization of the s electrons through $s-d$ hybridization.

The presence of the renormalization factor allows us to understand why, for transition-metal electrodes, majority electrons have higher conductance (tunneling rate) when minority d electrons have larger density of states at Fermi level ($E_{\mathbf{k}\downarrow} = \epsilon_{\mathrm{F}}$): minority electrons are more strongly hybridized (smaller $E^p_{\mathbf{k}\downarrow} - f^p_{\mathbf{k}\downarrow}$), which leads to *smaller* $Z^p_{\mathbf{k}\downarrow}$ in equation (22), and thereby smaller tunnel currents for minority s electrons.

4 Spin-polarized tunneling in a tight-binding description

From the proceeding sections, we realize that it is desirable to have more accurate descriptions of tunneling, *e.g.*, to obtain more accurate transfer matrix elements, equation (10), than those given by the WKB approximation equation (13). In particular, a spatially resolved treatment, *i.e.*, a local description of the bands, seems necessary. The tight-binding method developed by Caroli *et al.* [4] clearly serves this purpose. To ascertain which features of the transition metals are most important in producing JMR we extend Caroli's method to include the multiple bands at the Fermi level of the transition metals and their spin polarization [17].

Tunnel conductance is formulated in a tight binding model as

$$G = (e^2/\hbar) \int \mathrm{d}\epsilon \mathrm{Tr}(\rho_{\mathrm{L}}^{\alpha} t \rho_{\mathrm{R}}^{\beta} t^{+}) \tag{23}$$

where $\rho_{\mathrm{L}}^{\alpha}$ is the density of states at the surface α of the *isolated* left electrode, $\rho_{\mathrm{R}}^{\beta}$ that at the surface β of the *isolated* right electrode, and t is the renormalized transfer matrix which describes the coupling between the isolated left and right electrodes. These isolated systems are defined such that there is no transfer of electrons between them, *i.e.*, the Green's function G_{ij} is identically zero if i and j belong to different electrodes. As pointed out by Feuchtwang [18] this condition on the Green's function is not absolutely required to define isolated systems, however we find it convenient in deriving some meaningful relations.

There are two convenient ways to spatially define left and right systems. The first is for the left system to comprise the left electrode only and not to include the barrier region, and similarly for the right system; another way will be discussed later. In this case the density of states $\rho_{\mathrm{L}}^{\alpha}$ and $\rho_{\mathrm{R}}^{\beta}$ are density of states of at the surfaces of *isolated* electrodes. These density of states are *not* the physical ones at the interface of a metal-insulator or metal-vacuum contact; these latter quantities allow for charge to spill over from the metal into the insulator or vacuum, *i.e.*, $G_{ij} \neq 0$ for i in the electrode and j in the barrier, while the former quantities do not allow such leakage ($G_{ij} = 0$). With these left and right systems, one finds that the transfer matrix is

$$t = V_{\alpha a} G_{ab} V_{b\beta} \tag{24}$$

where

$$G_{ab} = \frac{g_{ab}}{(1 - V_{\alpha a}^2 g_{\alpha\alpha}^{\mathrm{L}} g_{aa})(1 - V_{b\beta}^2 g_{\beta\beta}^{\mathrm{R}} g_{bb}) - V_{\alpha a}^2 V_{b\beta}^2 g_{ab}^2 g_{aa} g_{bb}} \tag{25}$$

is the Green's function between plane a at the left end of the barrier (adjacent to α in the left electrode) and b at the right hand end (adjacent to β in the right electrode). The uncoupled Green's function for the insulator is g_{ab}, $V_{\alpha a}$ is the hopping matrix between α and a, and $V_{b\beta}$ is the hopping matrix between b and β. One might jump to the conclusion from equations (23-25) that the tunnel conductance is proportional to the density of the state at the interfaces, $\rho_{\mathrm{L}}^{\alpha}$ and $\rho_{\mathrm{R}}^{\beta}$; at least in the limit of weak interactions between the electrodes and insulator (small $V_{\alpha a}$ and $V_{b\beta}$). This conclusion is somewhat too rash for two reasons: the first is that the matrix element $V_{\alpha a}$ and $V_{b\beta}$ are expected in some way to depend on the density of states of the electrodes; the second is that the density of the states at the surface of an isolated electrode is not the physical density of the states of the surface of that electrode. While the first point is hard to address without lengthy *ab initio* calculations [11], we will now show the difference between the two density of states [19].

Let's assume a bulk electrode is separated into two identical isolated systems by slicing it midway between neighboring planes A and B. Then the Hamiltonian for the electrode is the sum of two isolated parts plus a hopping term V_{AB} between A and B. If one restricts hopping to nearest neighbors, V_{AB} represents hopping across the interface. If one considers hopping beyond nearest neighbors, A and B each represent multiple planes (supercell) and V_{AB} will be a supermatrix. The Green's function of the bulk electrode at A (actually any plane) is,

$$G_{\mathrm{AA}} = g_{\mathrm{AA}} + g_{\mathrm{AA}} V_{\mathrm{AB}} G_{\mathrm{BA}} \tag{26}$$

where

$$G_{\mathrm{BA}} = g_{\mathrm{BB}} V_{\mathrm{BA}} G_{\mathrm{AA}} \tag{27}$$

and g_{AA} and g_{BB} are the Green's functions at the surfaces of the left and right *isolated* systems. From symmetry $g_{\mathrm{AA}} = g_{\mathrm{BB}}$ and $V_{\mathrm{AB}} = V_{\mathrm{BA}} = V$, so that we find

$$G_{\mathrm{AA}} = g_{\mathrm{AA}}[1 - g_{\mathrm{AA}} V g_{\mathrm{AA}} V]^{-1}, \tag{28}$$

i.e., the Green's function of the bulk is directly related to the isolated interface Green's function g_{AA}. In the limit of weak hopping they become the same. Alternatively, one can express the isolated g_{AA} in terms of Green's function for the bulk by solving the above equations. By eliminating the hopping matrix from equations (26, 27), we find

$$g_{\mathrm{AA}} = (G_{\mathrm{AA}} G_{\mathrm{BA}}^{-1} - G_{\mathrm{BA}} G_{\mathrm{AA}}^{-1})(G_{\mathrm{BA}}^{-1} - G_{\mathrm{AA}}^{-1})^{-1}. \tag{29}$$

That is, the isolated Green's function g_{AA} and thereby the density of states ρ at the surface are solely determined by the Green's functions G_{AA} and G_{BA} of the bulk.

One concern one might have about the tight binding approach is whether the conductance depends on the choice of the isolated systems. In equation (23), it appears that conductance is related to the density of state at the *surface* of the electrodes. However, if one chooses for isolated systems the electrode each with half of the insulator-barrier, then equation (23) would imply that the conductance is related to the density of states at the middle of the insulator. In fact, when we take account of the weak hopping inside the insulator, we can show that this density of states is proportional to that at the surface

of the electrode. To see this we write down Dyson's equation in the limit of weak V as

$$g^{ii} = g_0^{ii} + g_0^{ii} V_{i,i-1} g^{i-1,i-1} V_{i-1,i} g_0^{ii}, \tag{30}$$

where i represents a plane in the middle of the insulator, $g_0^{ii} = (\epsilon - U)^{-1}$ is the Green's function of the isolated insulator (if the barrier is a vacuum U is the work function), g^{ii} is the Green's function of the isolated system defined as the left electrode with i layers of the insulator, and $g^{i-1,i-1}$ the Green's function of the isolated system defined as left electrode with $i-1$ layers of the insulator. Since g_0^{ii} is always real at the Fermi energy (for an insulator there are no states at the Fermi level), one finds that the density of states, which is the imaginary part of the Green's function, is

$$\rho^{ii} = [V g_0^{ii}]^2 \rho^{i-1,i-1}, \tag{31}$$

where we set $V_{i,i-1} = V_{i-1,i} \equiv V$. By repeatedly using this relation we find ρ^{ii} in terms of $\rho^{i-i,i-i} \equiv \rho^{ss}$, the density of states at the surface of the isolated electrode,

$$\rho^{ii} = \left(\frac{V}{\epsilon - U}\right)^{2i} \rho^{ss} \equiv \exp(-2k_{\rm b}t_{\rm b})\rho^{ss} \tag{32}$$

where $t_{\rm b}$ is the thickness of the insulator, and

$$k_{\rm b} = \frac{1}{2a_0} \ln(\frac{|\epsilon - U|}{V}) \tag{33}$$

where a_0 is the distance between atomic planes. Therefore the density of states at the center of the insulator is indeed proportional to density of states at the surface of the isolated electrode; the constant of proportionality is simply an exponentially decaying factor.

5 Effects of interface roughness

Up till now, we have not considered effects of disorder in magnetic tunnel junctions. However, actual junctions contain large amounts of disorder in the barriers as well as at interfaces with electrodes. When one compares theoretical models to experimental data, the effect of disorder must be taken into account.

Among other effects disorder introduces complex mechanisms that assist tunneling. At low temperatures contributions from impurity states in the barrier can be quite significant. As these states usually do *not* depend on spin, and as spin relaxation in these states is faster than the tunneling rate, their presence reduces magnetoresistance [20]. Also, effects of disorder *within* the insulator on tunneling and JMR has been recently considered by Tsymbal and Pettifor [21]. As detailed discussions of impurity assisted tunneling can be found in the book by Wolf [22], here we concentrate on disorder at interfaces, *i.e.*, interface roughness.

The simplest type of interface roughness is "geometric roughness", *i.e.*, fluctuations in layer thickness while the interface remains flat on an atomic length scale. In this case the local electronic structure does not deviate from that of an ordered structure of the same thickness, and tunnel conductance is simply the sum over the entire junction that is comprised of regions (areas) of different thicknesses. Due to the strong dependence of tunnel conductance on thickness of the barrier those areas which have smallest barrier thickness contribute most to conduction. To obtain a more quantitative estimate of the effects of geometric roughness we describe it's profile by a Gaussian distribution function, *i.e.*,

$$P(x) = \frac{1}{\sqrt{2\pi}\Delta} \exp\left[-\frac{(x-\bar{d})^2}{2\Delta^2}\right] \tag{34}$$

where $\bar{d}$ is the average thickness of the barrier and Δ is the root-mean-square deviation. The thickness dependence of tunnel conductance is proportional to $\exp(-2k_{\rm b}x)$, *e.g.*, see equation (2), so that the average of the conductance over the above distribution of thicknesses is proportional to

$$\bar{G}(\bar{d}) \propto \int P(x)\exp(-2k_{\rm b}x){\rm d}x = \exp\left(-2k_{\rm b}[\bar{d} - k_{\rm b}\Delta^2]\right). \tag{35}$$

The effect of this geometrical roughness is expressed by a reduction in the nominal thickness of the barrier by $k_{\rm b}\Delta^2$. Therefore, the barrier thickness found by fitting $I-V$ characteristics of a junction to Simmon's formula yields an effective thickness which depends on the roughness.

Other forms of roughness, such as interdiffusion, dislocations, stacking faults and vacancies at interfaces, influence JMR in more complicated ways. Electronic structure at an interface is significantly altered by these types of roughness. As we have seen in previous sections, tunnel magnetoresistance and conductance depend critically on details of this structure and the concomitant hopping across such imperfect interfaces. At present it is difficult to perform first principle calculations which include these effects, therefore phenomenological approaches are more realistic. One approach, first taken by Caroli [4], is to average over $k_{||}$ the density of states and transfer matrices entering the conductance so that one is left with a one dimensional integral over energy, see equation (23); at low temperatures this reduces to evaluating these components at the Fermi energy. One can also represent the diffuse scattering at interfaces due to interfacial roughness by a delta function whose strength is given by a phenomenological parameter ξ_i as was done in our derivation of equation (7); by fitting this expression to data on different electrodes and barriers we are able to determine ξ_i. Finally, Itoh *et al.* [23] took account of "strong disorder" by expressing tunnel conductance in terms of phenomenological self-energies for the interfaces.

In concluding this section we note that the effects of interface roughness on JMR are dramatic; yet only crude phenomenological approaches are presently available to deal with it.

6 Discussion

We have outlined three models for the magnetoresistance of tunnel junctions: the free electron one band model with a chosen profile of the potential barrier; the transfer Hamiltonian method with a transfer matrix elements given by the WKB approximation; and the tight-binding description of tunneling. Here we summarizes their advantages and deficiencies.

While tunnel conductance can be exactly calculated for a given potential profile in the free electron model the JMR derived from this approach is not reliable, because magnetoresistance is sensitive to the profile of the potential barrier. Approximations such as δ function-like potentials at interfaces and a square barrier for the insulating layer dramatically change the prediction for the JMR. Due to the arbitrariness in choosing the potential profiles, this method is unreliable for estimating the magnetoresistance of tunnel junctions. However, this approach is easy and physically transparent; it correctly gives the exponential decay of the current with the thickness of the barrier. It strength lies in the simplicity of the assumed potential profile and band structure; it is useful much as Simmon's formula is useful in analyzing the $I-V$ characteristics of tunnel junctions.

The transfer Hamiltonian is a many-body description of the tunneling, inasmuch as it contains several bands at the Fermi level, and hybridization between them. The difficulty of this approach is the ill-defined transfer matrix elements; usually they are considered as phenomenological parameters. By using the WKB approximation one is able to link these matrix elements to the electronic structure of the electrodes, see equation (13); however, this approximation is questionable because the potential changes rapidly between the electrode and barrier on the length scale of the wavelength of the carriers at the Fermi surface. As we showed in Section 3 if we suppress tunneling by d electrons it is possible to explain the positive spin-polarized current seen by experiments with transition-metal electrodes without additional assumptions. Another advantage of this approach is that one can include a number of inelastic physical excitations into the tunneling process [24]. We have shown previously that surface magnon-assisted tunneling can be easily dealt with within this approach [25]; other inelastic processes, such as the effects of trapped impurity states and localized phonons, can be included on an equal footing to those we considered.

The tight-binding approach relates tunnel conductance and magnetoresistance to electronic structures for isolated electrodes and to the hopping matrix elements between electrodes and the insulator. The electronic structures of the isolated electrodes can be accurately determined from the bulk properties of the electrodes. Some predictions can be made with this method. For example, in the limit of weak and spin independent hopping between the electrodes and the insulator, tunnel conductance and magnetoresistance are related to the density of states of the *bulk* electrodes. This method is capable of taking into account realistic electronic structures. Moreover, since this approach emphasizes local electronic structure, it is quite possible to deal with more complicated junctions, *e.g.*, inserting a thin metal layer at the interface. However, to obtain reliable information from this approach one needs to know details of the hopping matrix elements such as: the relative strengths of the $s-p$ and d electron hopping, the range of the hopping, whether its limited to the first few nearest neighbors or not, and the spin dependence of the hopping [17]. At this time these details are not known for Al_2O_3, the insulator used in many tunnel junctions; therefore, it would be serendipitous if the theoretically determined magnetoresistance agreed with experimental data.

We are currently at the stage of qualitatively understanding some features of magnetic tunnel junctions that control their magnetoresistance, *e.g.*, that JMR is related to the itinerant density of states of the electrodes. All of the methods we considered suffers a common drawback: the need to know details about the coupling between electrodes and the insulator; these are poorly known at the present time for the junctions that have been studied. It is very difficult at this time to do *ab initio* calculations for junctions with an insulator such as alumina; albeit, a first step in this direction has been taken [26]. Therefore, it is interesting to examine simpler systems, *e.g.*, by replacing the real insulating barrier by a vacuum spacer [11,27]. The advantage of this simple system is that *ab initio* calculations are now possible; some of the features of tunneling through a vacuum barrier may well be similar to those when one uses alumina or other insulating spacer materials. Also, such a calculation is directly applicable to data on spin-polarized field emission experiments where there is truly a vacuum. The results of these calculations for a vacuum spacer will be published elsewhere [11].

This research was supported by the Office of Naval Research (N00014-96-1-0203), together with the Defense Advanced Research Projects Agency (DARPA-ONR N00014-96-1-1207) and (MDA972-96-C-0014). P.M.L. thanks Professor Albert Fert and the Laboratoire de Physique des Solides in Orsay, France for their hospitality during his sabbatical stay there.

References

1. T. Miyazaki, N. Tezuka, J. Magn. Magn. Mater. **139**, L231 (1995).
2. J.S. Moodera, L.R. Kinder, T.M. Wong, R. Meservey, Phys. Rev. Lett. **74**, 3273 (1995).
3. J.C. Slonczewski, Phys. Rev. B **39**, 6995 (1989).
4. C. Caroli, R. Combescot, P. Nozières, D. Saint-James, J. Phys. C: Solid State Phys. **4**, 916 (1971).
5. G.E. Blonder, M. Tinkham, T.M. Klapwijk, Phys. Rev. B **25**, 4515 (1982).
6. M. Sharma, S.X. Wang, J. Nickel (private communication).
7. J.S. Moodera, L.R. Kinder, J. Appl. Phys. **79**, 4724 (1996), Bull. Amer. Phys. Soc. **40**, 352 (1998); J.S. Moodera, M.E. Taylor, R. Meservey, Phys. Rev. B **40**, 11 980 (1989).
8. S. Zhang, P.M. Levy, Phys. Rev. Lett. **81**, 5660 (1998).
9. R. Meservey, P.M. Tedrow, Phys. Rep. **238**, 173 (1994).
10. J. Bardeen, Phys. Rev. Lett. **6**, 57 (1961).

11. K. Wang, S. Zhang, P.M. Levy (to be published).
12. W.A. Harrison, Phys. Rev. **123**, 85 (1961).
13. M.H. Cohen, L.M. Falicov, J.C. Phillips, Phys. Rev. Lett. **8**, 316 (1962).
14. M.B. Stearns, J. Magn. Magn. Mater. **5**, 167 (1977).
15. J.A. Hertz, K. Aoi, Phys. Rev. B **8**, 3252 (1973).
16. G.D. Mahan, in *Many-Particle Physics* (Plenum Press, New York and London, 1990).
17. The recent work by E.Yu. Tsymbal, D.G. Pettifor, J. Phys. Cond. Mater. **9**, L411 (1997) stressed the sensitivity of the MR in tunnel junctions to the electron bonding at the metal insulator interface.
18. T.E. Feuchtwang, Phys. Rev. B **10**, 4121, 4135 (1974).
19. See J. Pollmann, S.T. Pantelides, Phys. Rev. B **18**, 5524 (1978) for methods of calculating surface Green's functions.
20. J. Zhang, R.M. White, J. Appl. Phys. **83**, 6512 (1998).
21. E.Yu. Tsymbal, D.G. Pettifor, Phys. Rev. B **58**, 432 (1998).
22. E.L. Wolf, in *Principles of Electron Tunneling Spectroscopy* (Oxford University Press, Oxford, 1985).
23. H. Itoh, A. Shibata, T. Kumazaki, J. Inoue, S. Maekawa, J. Phys. Soc. Jap. **68**, 5 (1999).
24. C.B. Duke, in *Tunnelling in Solids* (Academic Press, New York, 1969).
25. S. Zhang, P.M. Levy, A.C. Marley, S.S.P. Parkin, Phys. Rev. Lett. **79**, 3744 (1997).
26. D. Nguyen-Manh, E.Yu. Tsymbal, D.G. Pettifor, C. Arcangeli, R. Tank, O.K. Andersen, A. Pasturel, MRS Symp. Proc. **492**, 319 (1998).
27. J.M. MacLaren, X.-G. Zhang, W.H. Butler, Phys. Rev. B **56**, 11 827 (1997).