Low Voltage I-V Characteristics in Magnetic Tunnel Junctions

G. G. Cabrera

Instituto de Física ‘Gleb Wataghin’,
Universidade Estadual de Campinas (UNICAMP),
C. P. 6165, Campinas 13.083-970 SP, Brazil

and

N. García

Laboratorio de Física de Sistemas Pequeños y Nanotecnología,
Consejo Superior de Investigaciones Científicas (CSIC),
Serrano 144, E-28006 Madrid, Spain
(November, 2000)

Abstract

We show that elastic currents that take into account variations of the tunnel transmittivity with voltage and a large ratio of majority to minority spin densities of states of the $s$ band, can account for the low voltage current anomalies observed in magnet-oxide-magnet junctions. The anomalies can be positive, negative or have a mixed form, depending of the position of the Fermi level in the $s$ band, in agreement with observations. Magnon contribution is negligible small to account for the sharp drop of the magnetoresistance with the voltage bias.
Tunneling of electrons in metal-insulator-metal junctions is an old phenomenon studied from a long time ago [2,3]. However, it is only quite recently that spin-dependent tunneling between two ferromagnetic metals has been shown to produce the magnetoresistance effect observed in those systems [4,5]. In 3d ferromagnets, most of the spin polarization comes from the d bands, while tunneling currents are dominated by s band contributions. This is so, because d wave functions are more localized and their effective tunneling barrier is higher [6]. For Ni, it has been estimated that the tunneling probability of the s electrons is of the order of 100 – 1000 times that of the d electrons, thus leading to a positive spin polarization in Ni field emission experiments [4]. In the context of tunneling experiments, the large magnetoresistance effect (25-30 %) found in [4,5] is puzzling, since it points to a large polarization of the s band, with a ratio of the densities of states for majority \( N^M(E_F) \) and minority \( N^m(E_F) \) electrons at the Fermi level \( E_F \) of the order of
\[
N^M(E_F)/N^m(E_F) \approx 2.0 – 2.5, \tag{1}
\]
in apparent contradiction with energy band calculations for ferromagnetic metals [8].

In addition, a remarkable dependence of the junction conductance with the voltage bias \( V \) has been observed at low voltages (of the order of a few hundred millivolts). As usual in magnetoresistance experiments, one compares the resistances for the cases where the magnetizations at the electrodes are anti-parallel (AP) and parallel (P). In several experiments reported in Ref. [4,5], the junction resistance drops significantly with the applied voltage, with a peak at zero bias (called zero-bias anomaly) that is more pronounced for the AP alignment. The effect is also temperature dependent, the peak being less sharp at room temperature. Finally, it is found that the junction magnetoresistance (JMR) has a large decrease with voltages, up to 60% at 0.5 V in some cases [4]. It has been argued that this effect can be attributed to the excitation of internal degrees of freedom by hot electrons (even at liquid He temperature). Scattering from surface magnons has been proposed as a mechanism to randomize the tunneling process and open the spin-flip channels that leads eventually to a sharp drop of the MR [5]. However, this explanation is controversial, since magnon scattering cross sections are negligibly small to account for such a big drop of resistance and no spin-flip events have been observed in experiments with polarized injected electrons in tunnelling phenomena [5]. Also, the theory given in Ref. [5] assumes tunneling transmitivities independent of the applied voltages, and uses a perturbation scheme only valid for voltages smaller than \( \sim 40 \, \text{mV} \), while the data extend to \( \sim 400 \, \text{mV} \).

In the present Letter, we show that the variations of the conductance with the voltage bias can be simply accounted for by the lowering of the barrier height with voltages, as given by the Simmons’ tunneling theory [3]. The structure at zero bias is obtained, when one properly takes into account variations of the density of states with the bias at both magnetic electrodes. Assuming that the tunneling current comes from the s band, we formulate a simple model with a parabolic dispersion (free-electron like). We obtain different behaviors for the zero-bias anomaly, whether the Fermi level is located near the bottom (peak) or top of the band (dip). Fitting with the experiments [4,5] can only be obtained if one assumes a large spin polarization corresponding to relation (1).

In order to develop our calculation, one has to rewrite Simmons’ formulae with the conductance current written in the form
\[ J^{(C)}(V) = A \sum_{\sigma, \mu} \int_{-\infty}^{\infty} dE \ T(E, \Delta s, \phi, V) \ N_L^{(\sigma)}(E) N_R^{(\mu)}(E + V) \left[ f_L(E) - f_R(E + V) \right] , \quad (2) \]

where \( T(E, \Delta s, \phi, V) \) is the transmittivity through the barrier for energy \( E \), parametrized with the mean barrier height \( \phi \) and width \( \Delta s \) \(^3\), the index \( C = P, AP \) refers to the magnetic configuration (parallel or anti-parallel), and \( N_{L,R} \) and \( f_{L,R} \) are the densities of states and the Fermi distributions for the left and right electrodes, respectively. In ferromagnets, one has to distinguish between majority \((M)\) and minority \((m)\) spin bands and the super-indices \( \sigma, \mu \) in the densities of states and in the sum in expression (2) label the allowed processes for spin conserving tunneling, for both magnetic configuration, \( P \) and \( AP \). For parallel alignment, the factor of the densities of states that enter in (2) is

\[ N_m^{(M)}(E) N_m^{(M)}(E + V) + N_m^{(M)}(E) N_m^{(M)}(E + V) , \quad (3) \]

while for the anti-parallel configuration, where majority and minority are interchanged for the left and right electrodes, one has to consider

\[ N_m^{(M)}(E) N_m^{(M)}(E + V) + N_m^{(M)}(E) N_m^{(M)}(E + V) . \quad (4) \]

Concerning equation (2), several remarks are in order.

i) In his original treatment of the tunneling problem \(^3\), Simmons considers the case of very flat conduction bands for the metal electrodes and takes the densities of states as constants. However, for \( s \) bands the density of states varies as the square root of the energy, and for magnetic junctions this cannot be neglected, especially near the band edges, where the variation is bigger. Zero-bias anomalies in normal non-magnetic metals has been previously reported, in cases where the structure of the density of state is important \(^11\).

ii) Expression (2) involves an integral over all energies, but states that are deep in the band are cut off exponentially by the tunneling probability. As a net result, the conductance is dominated by electrons that are near the Fermi level, and (2) approximately factorizes in the form

\[ J^{(C)}(V) \approx \left( \sum_{\sigma, \mu = m, M} C N^{(\sigma)}(E_F) N^{(\mu)}(E_F + V) \right) J^{(S)}(V) = D^{(C)}(E_F, V) \ J^{(S)}(V) \quad (5) \]

where \( J^{(S)}(V) \) is the Simmons’ tunneling current as a function of the voltage bias and

\[ D^{(C)}(E_F, V) = \sum_{\sigma, \mu = m, M} C N^{(\sigma)}(E_F) N^{(\mu)}(E_F + V) . \quad (6) \]

In (3), we are assuming that both electrodes are made from the same ferromagnetic metal. The term \( J^{(S)}(V) \) is the Simmons’ contribution, is spin independent and carries all the information concerning the tunneling barrier. As shown in \(^3\), it has no quadratic term in the voltage for small bias, and no zero-bias anomaly.
In Fig. 1, we show the variation with voltage of the Simmons resistance for typical barriers, with the resistance normalized at zero bias. A large variation is observed in all the examples, but the resistance has no peak or dip at zero voltage. Except for the structure at zero bias, the overall variation of the Simmons’ resistance is of the order of what is observed in experiments (or even may vary faster with voltage in some cases). Some experimental results are also shown for comparison.

Next, we introduce the factor $D^{(C)}(E_F, V)$, defined in (6), in the conductance calculation. We model the density of states of the $s$ bands with a parabolic dependence (free-electron like) in the form

$$N^{(\sigma)}(E) = \frac{\Omega}{4\pi^2} \left( \frac{2m_e}{\hbar^2} \right)^{3/2} \sqrt{\pm (E - E_\sigma)}, \quad \sigma = m, M,$$

where $\Omega$ is the volume of the sample (electrode), $m_e$ is the electron mass, and the $\pm$ sign refers to the cases where we are in the bottom or in the top of the conduction band, respectively. In formulating the Stoner model within a naive band theory, $|E_m - E_M|$ should yield the exchange of the $s$ band. But Fermi surfaces of transition metals are very intricate, with contributions from electron and hole-like carriers and with different shapes for majority and minority spin sheets. In this context, $E_m$ and $E_M$ come from the band structure and $\Delta E = |E_m - E_M|$ may be very different from the true exchange of the band.

To parametrize our results, and denoting by $E_F$ the Fermi energy, we define

$$E^M_F \equiv |E_F - E_M|,$$
$$E^m_F \equiv |E_F - E_m|,$$
$$E^M_F \equiv \lambda E^m_F, \quad \lambda > 1,$$

which includes both cases, bottom and top of the band. The ratio of the densities of states at the Fermi level is given by $N^{(M)}_L(E_F)/N^{(m)}_L(E_F) = \sqrt{\lambda}$. Several possibilities can be realized, whether majority and minority carriers are electrons or holes. When both are electrons or holes, the factors $D^{(C)}(E_F, V)$ can be expanded in series in $V$, yielding a linear term in $V$ that is responsible for the zero-bias anomaly:

$$D^{(P)}_\pm (V) \approx \left( \left[ N^{(m)}(E_F) \right]^2 + \left[ N^{(M)}(E_F) \right]^2 \right) \left( 1 \pm p^{(P)} |V| \right),$$
$$D^{(AP)}_\pm (V) \approx \left( 2N^{(m)}(E_F)N^{(M)}(E_F) \right) \left( 1 \pm p^{(AP)} |V| \right),$$

where the $\pm$ sign labels the bottom and top cases respectively, with the slopes of the linear terms given by

$$p^{(P)} = \frac{1}{E^m_F (1 + \lambda)} ,$$
$$p^{(AP)} = \frac{\lambda + 1}{4\lambda E^m_F} .$$

When we have a mixed case, i.e. one of the spin is electron-like and the other hole-like, no linear term appears in $D^{(P)}(V)$. On the other hand, for $D^{(AP)}(V)$, the slope of the linear term is given by
\[ p^{(AP)} = \mp \left( \frac{\lambda - 1}{4\lambda E_m^F} \right), \]

where the \(-\) (\(+\)) sign applies when the majority carriers are electrons (holes). In Fig. 2, we display results of our calculation for examples of typical barriers. The value of the magnetoresistance at zero bias was taken from Ref. [5], with

\[ N^{(M)}_L(E_F)/N^{(m)}_L(E_F) = \sqrt{\lambda} \approx 2.2. \]

In Fig. 2 a), we show the case when the Fermi level is in the bottom of the \(s\) band, with a linear decrease of the resistance with the voltage bias for both magnetic configurations (\(AP\) and \(P\)). If the Fermi level is in the top of both spin bands, we initially get a linear increase of the resistance which, after some voltage value, is dominated by the Simmons’ term. This case is displayed in part c) of Fig. 2. In Fig. 2 b), we display the situation where the majority band (\(\uparrow\)) is almost filled (holes) and the minority (\(\downarrow\)) is almost empty (electrons). The resistance for the \(P\) setup, exhibits no linear term. In Fig. 2 a), we also show experimental results taken from Ref. [5]. We have not tried an optimum fitting with experiments, but it is clear that experimental results can only be explained assuming a large polarization of the \(s\) band. Note that the insets in Fig. 2 a)-2 c) sketch the band configurations for both spins.

The change in tunnel resistance or magnetoresistance (MR) is given by

\[ \frac{\Delta R}{R} = \frac{R_{AP} - R_P}{R_{AP}}, \tag{7} \]

where again, \(AP\) and \(P\) refer to the magnetic configuration of the ferromagnetic electrodes. This ratio, as it is evident from relation (7), is almost independent of the Simmons’ term, not depending on details of the tunneling process. In Fig. 3 A), we display results of \(\Delta R/R\) corresponding to the examples of Fig. 2. In B), we take different experimental results found in the literature [4]. Note that when the Fermi level lies near the top of the band, there is an increase of the MR. Eventually, we may reach the minority spin band edge, with a vanishing density of states, for which

\[ R_{AP} \rightarrow \infty. \]

Temperature \((T)\) effects can also be taken into account through relation (2), with the broadening of the Fermi distributions, but a rough estimation shows that the effect should be similar to that of an applied voltage \(V \approx 2T\), with an effective lowering of the barrier height, a smaller resistance, and the softening of the zero-bias anomaly, in agreement with experiments.

From our calculations presented above the following conclusions are pertinent:

i) The overall variation of the tunnel current with voltage [4,5] can be explained by elastic tunneling using the well known Simmons’ formula [3] and is due to the lowering of the barrier by the applied voltage. This is at variance with the calculations in Ref. [4], where they argue that this effect is negligible. Therefore, magnons are not needed to explain the experiments;
ii) The anomalies in the currents and the magnetoresistances can be explained within this simple framework, provided that the ratio of majority spin to minority spin electrons is of the order of $2.2 - 2.5$, for the data of Ref. [4,5]. If one is allowed to choose the adequate configuration of the s bands (see Fig.2), a maximum, a minimum or a mix of both can appear at the anomaly (as it has been observed in Ref. [11]);

iii) From band structures calculations [8], it is not clear to us that the above polarization of the s band can be justified. There may be other oxidation states inside the metal, at the interface, and in the oxide layer, that contribute to the polarization of the current;

iv) Alternatively, it may also happen, as it has been suggested in Ref. [8,12,13], that the current is dominated by conduction paths that provide large values of magnetoresistance [14] due to domain wall scattering [15], and then there is also contribution of $d$-electrons. In this case, the density of states will have mixed contributions from s and d-electrons, with a variety of topologies in the MR [16];

v) The main conclusion is that the magnetoresistance is a mapping of the spin up and down densities of states in the metals and the barrier and cannot be assigned only to the bulk ferromagnetic metals, and many mixing possibilities exist for explaining the physical measurements.

Acknowledgments. GGC acknowledges partial support from Brazilian FAPESP (Fundação de Amparo à Pesquisa do Estado de São Paulo) and CNPq (Conselho Nacional de Desenvolvimento Científico e Tecnológico).
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FIGURE CAPTIONS

Fig. 1 Variation of the Simmons’ resistance with voltage for several tunnel barriers. Data is normalized at zero bias. Experimental results from [3] are also shown (solid triangles) as a reference.

Fig. 2 Resistance as a function of the voltage bias for the two configurations of the magnetic electrodes and for different $s$ band structures (they are shown in the insets). Parameters for the tunneling barriers are given in each figure. Spin $\uparrow$ is taken as the majority band in all cases. As a reference, experimental results take from [3] are shown in part a), where a good agreement with our calculation is obtained.

Fig. 3 Magnetoresistance, as defined in (3), for all the cases depicted in Fig. 2. Densities of states are adjusted at the zero bias value. In A), we compare with results from [3], while part B) compares with Ref. [4].
Fig. 1

- Resistance (normalized at zero bias) vs. Junction Bias (Volts)
- Curves for different angles: 10°, 20°, 30°
- Solid line for $\phi = 2.0$ eV
- Dashed line for $\phi = 1.5$ eV
- Exp. points

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Fig. 2

(a) $E_F^m = 0.7 \text{ eV}$
- $s = 10 \ A^0$, $\phi = 2.0 \text{ eV}$

(b) $E_F^m = 0.3 \text{ eV}$
- $s = 13 \ A^0$, $\phi = 1.5 \text{ eV}$

(c) $E_F^m = 0.7 \text{ eV}$
- $s = 20 \ A^0$, $\phi = 2.0 \text{ eV}$

Resistance (normalized at zero bias)

Junction Bias (Volts)
Fig. 3

(A) Magnetoresistance (%)

![Graph A](image)

- Ref. 5

(B) Junction Bias (Volts)

![Graph B](image)

- Ref. 4

Fig. 3