Chapter 10

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ELEG/PHYS667 Magnetism & Spintronics
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The next topic we will cover is Tunnel Magneto-Resistance (TMR) which is the result of transport perpendicular to the film plane, where the normal metal conductive spacer between the ferromagnetic layers is replaced with an insulator. The insulator is a barrier for electrons which can "quantum-mechanically" tunnel through it. Before discussing TMR, we need to understand the details of electron tunneling.

1 Simmons tunneling model

The number of electrons going from electrode 1 (on the left) to 2 (on the right) is given by the total contribution of the product of particle flux and transmission probability from every state in the Fermi sphere.

1.1

What is the single-particle contribution to the particle flux? We can start by looking for a continuity equation of the form

$$\frac{d}{dt}P = \bigtriangledown \cdot J \tag{1}$$

Where P is particle density. In quantum mechanics, we know $P = \Psi^*\Psi$, so we can derive J, the particle current, starting from the left hand side.

$$\frac{d}{dt}P = \frac{d}{dt}\Psi^*\Psi = \frac{d\Psi^*}{dt}\Psi + \Psi^*\frac{d\Psi}{dt} \tag{2}$$

and we can use the Schrödinger equation and its conjugate to evaluate the time derivatives

$$\frac{-\hbar^2}{2m}\bigtriangledown^2 \Psi + V\Psi = i\hbar\frac{d\Psi}{dt} \tag{3}$$

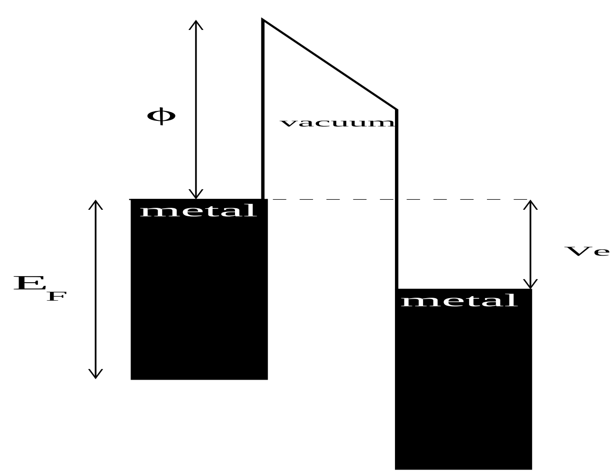


Figure 1: Schematic tunnel junction energy diagram.

$$\frac{-\hbar^2}{2m}\bigtriangledown^2\Psi^* + V\Psi^* = -i\hbar\frac{d\Psi^*}{dt} \tag{4}$$

giving

$$\frac{d}{dt}P = (-\frac{i\hbar}{2m}\bigtriangledown^2\Psi^* + \frac{i}{\hbar}V\Psi^*)\Psi + \Psi^*(\frac{i\hbar}{2m}\bigtriangledown^2\Psi^* - \frac{i}{\hbar}V\Psi^*) \tag{5}$$

The potential energy terms cancel and we have

$$= \frac{i\hbar}{2m}\left(\Psi^*(\bigtriangledown^2\Psi) - (\bigtriangledown^2\Psi^*)\Psi\right) \tag{6}$$

Now add and subtract a term

$$= \frac{\hbar}{2im}\left(\Psi^*(\bigtriangledown^2\Psi) + \frac{d}{dx}\Psi^*\frac{d}{dx}\Psi - (\bigtriangledown^2\Psi^*)\Psi - \frac{d}{dx}\Psi^*\frac{d}{dx}\Psi\right) \tag{7}$$

Which allows us to extract a $\bigtriangledown$:

$$= \bigtriangledown\cdot\left[\frac{\hbar}{2im}\left((\bigtriangledown\Psi^*)\Psi - \Psi^*(\bigtriangledown\Psi)\right)\right] = \bigtriangledown\cdot J \tag{8}$$

The term in brackets can now be identified with the particle current density (flux).

1.2 Particle Current density for plane-waves

Since we want to calculate total current density contributed by all the states in the Fermi Sphere, we can apply this expression to individual plane-wave states

$$\Psi = e^{ik\cdot r} \tag{9}$$

$$J = \frac{\hbar}{2im}\left(\Psi^*(\bigtriangledown\Psi) - (\bigtriangledown\Psi^*)\Psi\right) \tag{10}$$

$$J = \frac{\hbar}{2im}\left(\Psi^*(ik\Psi) - (-ik)\Psi^*\Psi\right) = \frac{\hbar k}{m} \tag{11}$$

So the particle current density is the momentum $\hbar k$ divided by the mass... that equals velocity! Therefore, the flux of particles (electrons with plane-wave wavefunctions) through a plane is the velocity component perpendicular to that plane.

1.3 Integration Over Fermi Sphere

The flux is given by the state's perpendicular velocity, but we must also take into account the Pauli exclusion principle; only states which are filled in the metal on the left that have states with equal energy on the right that are unoccupied can contribute. Therefore,

$$N_1 = \frac{2}{(2\pi)^3}\int\frac{p_z}{m}f_1(E)[1 - f_2(E + eV)]T(E_z)\frac{d^3p}{\hbar^3} \tag{12}$$

where the $f()$'s denote Fermi-Dirac functions and $T(E_z)$ is the transmission probability. We would like to do the integral over energy, not momentum. Using $dE_z = \frac{\hbar}{m}p_z dp_z$, we can write

$$N_1 = \int_0^{E_F} T(E_z)n(p_z)dE_z \tag{13}$$

if

$$n(p_z) = \frac{1}{4\pi^3}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} f_1(E)[1 - f_2(E + eV)]\frac{dp_x dp_y}{\hbar^3}. \tag{14}$$

We can evaluate this integral by using

$$E = E_r + E_z \tag{15}$$

$$E_r = \frac{p_x^2 + p_y^2}{2m} = \frac{p_r^2}{2m} \tag{16}$$

$$E_z = \frac{p_z^2}{2m} \tag{17}$$

If we change variables to $p_x = p_r \cos\theta$ and $p_y = p_r \sin\theta$, we have

$$n(p_z) = \frac{1}{4\pi^3} \int_0^{2\pi} \int_0^{\infty} f_1(E)[1 - f_2(E + eV)] p_r \frac{dp_r d\theta}{\hbar^3} \tag{18}$$

now since $dE_r = \frac{p_r dp_r}{m}$, $dp_r = \frac{m}{p_r} dE$ so

$$n(p_z) = \frac{m}{2\pi^2\hbar^3} \int_0^{\infty} f_1(E)[1 - f_2(E + eV)] dE_r \tag{19}$$

$$N_1 = \frac{m}{2\pi^2\hbar^3} \int_0^{E_F} T(E_z) dE_z \int_0^{\infty} f_1(E_z + E_r)[1 - f_2(E_z + E_r + eV)] dE_r \tag{20}$$

There is also a particle flux moving from right to left:

$$N_2 = \frac{m}{2\pi^2\hbar^3} \int_0^{E_F} T(E_z) dE_z \int_0^{\infty} f_2(E_z + E_r + eV)[1 - f_1(E_z + E_r)] dE_r \tag{21}$$

The total current density is $J = -e(N_1 - N_2)$,
If

$$\xi_1(E_z) = \frac{me}{2\pi^2\hbar^3} \int_0^{\infty} f_1(E)[1 - f_2(E + eV)] dE_r \tag{22}$$

$$\xi_2(E_z) = \frac{me}{2\pi^2\hbar^3} \int_0^{\infty} f_2(E + eV)[1 - f_1(E)] dE_r \tag{23}$$

and

$$\xi = \xi_1 - \xi_2 = \frac{me}{2\pi^2\hbar^3} \int_0^{\infty} [f_1(E) - f_2(E + ev)] dE_r \tag{24}$$

then

$$J = \int_0^{E_F} T(E_z) \xi(E_z, eV) dE_z \tag{25}$$

1.4 Density of tunneling states

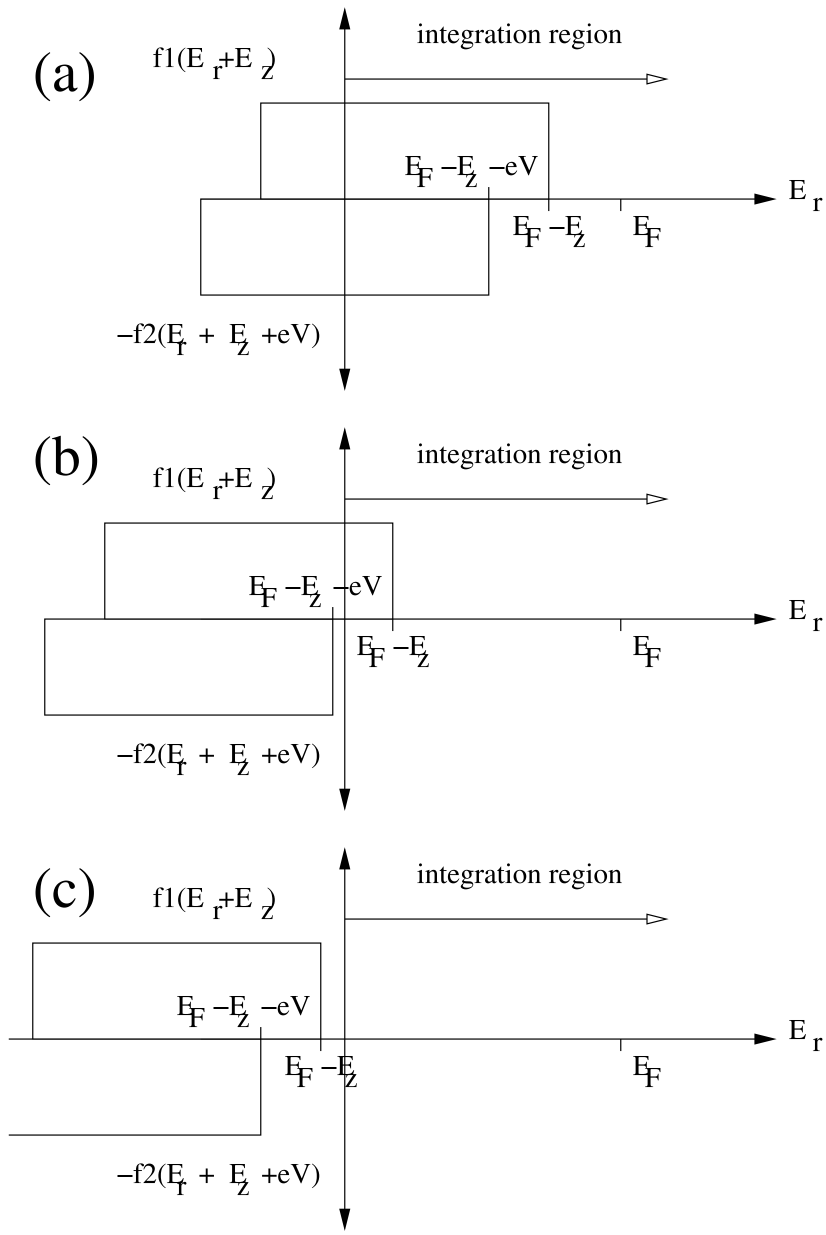
Now all we have to do is evaluate ξ and the tunneling transmission probability. Refer to the figure illustrating the integration region and the two functions.

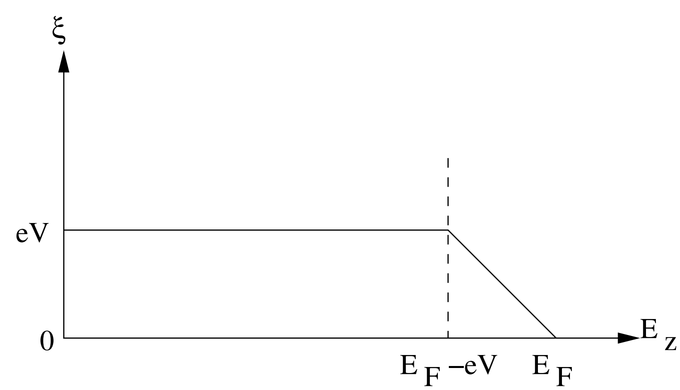
1.4.1 case a: $E_z < E_F - eV$

$$\frac{me}{2\pi^2\hbar^3} \int_0^{\infty} [f_1(E) - f_2(E + ev)] dE_r = (E_F - E_z) - (E_F - E_z - eV) = eV \tag{26}$$

1.4.2 case b: $E_F - eV < E_z < E_F$

$$\frac{me}{2\pi^2\hbar^3} \int_0^{\infty} [f_1(E) - f_2(E + ev)] dE_r = E_F - E_z \tag{27}$$


(a)
f1(E r+E z)
integration region
E F −E z −eV
E F −E z
E F
E r
−f2(E r + E z +eV)
(b)
f1(E r+E z)
integration region
E F −E z −eV
E F −E z
E F
E r
−f2(E r + E z +eV)
(c)
f1(E r+E z)
integration region
E F −E z −eV
E F −E z
E F
E r
−f2(E r + E z +eV)


ξ
eV
0
E F −eV
E F
E z

1.4.3 case a:$E_z > E_F$

$$\frac{me}{2\pi^2\hbar^3}\int_0^\infty [f_1(E) - f_2(E+ev)]dE_r = 0 \tag{28}$$

Clearly, when $eV << E_F$, this tunneling density of states is approximately just a constant equal to eV. Therefore, the integral determining the current density J is just an integral over the tunneling probability times eV. The former does not change to first order, so we can conclude that for low bias, the tunnel junction appears ohmic.

1.5 WKB theory

We need to get an expression for the tunnel transmission probability. The WKB (Wentzel-Kramers-Brillouin) method is a useful approximation.

We start with the time-independent 1-dimensional Schrödinger equation,

$$\left(\frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right)\Psi = E\Psi. \tag{29}$$

Since the solution, Ψ, to this equation is, in general, a complex function, we can make the generalization to "polar" form

$$\Psi = A(x)e^{i\phi(x)}, \tag{30}$$

where both $A(x)$ and $\phi(x)$ are real functions of x. In this form, the second derivative has the following effect:

$$\frac{d^2\Psi}{dx^2} = (A'' + 2iA'\phi' + iA\phi'' - A(\phi')^2)e^{i\phi}, \tag{31}$$

where the primes denote derivatives with respect to x.

If we now make the substitution $p = \sqrt{2m(E - V(x))}$, the Schrödinger equation becomes

$$\frac{d^2\Psi}{dx^2} = -\frac{p^2}{\hbar^2}\Psi. \tag{32}$$

Substitution of our ansatz yields

$$(A'' + 2iA'\phi' + iA\phi'' - A(\phi')^2)e^{i\phi} = -\frac{p^2}{\hbar^2}Ae^{i\phi} \tag{33}$$

$$(A'' + 2iA'\phi' + iA\phi'' - A(\phi')^2) = -\frac{p^2}{\hbar^2}A \tag{34}$$

This can be broken up into two equations, one for the real part and one for the imaginary part:

$$A'' - A(\phi')^2 = -\frac{p^2}{\hbar^2}A, \tag{35}$$

and

$$2iA'\phi' + iA\phi'' = 0. \tag{36}$$

The second equation is solved easily by noticing that $i(A^2\phi')' = A(2iA'\phi' + iA\phi'')$. We then have

$$(A^2\phi')' = 0. \tag{37}$$

This has solution $A = \frac{C}{\sqrt{\phi'}}$, where C is an undetermined constant, which is fixed by the boundary conditions and the unity probability restriction,

$$\int_{-\infty}^{\infty} \Psi^*\Psi dx = 1. \tag{38}$$

The first equation is more difficult to solve. However, by making the approximation that A is slowly-varying, the second-derivative of A is neglected to find

$$-(\phi')^2 = -\frac{p^2}{\hbar^2}, \tag{39}$$

which has solution

$$\phi(x) = \pm\frac{1}{\hbar}\int p(x)dx. \tag{40}$$

The WKB wavefunction is then

$$\Psi(x) = \frac{C_1}{\sqrt{p(x)}}e^{\frac{i}{\hbar}\int p(x)dx} + \frac{C_2}{\sqrt{p(x)}}e^{-\frac{i}{\hbar}\int p(x)dx}. \tag{41}$$

When we use this method for tunneling phenomena, the momentum, $p(x)$ is imaginary since $E < V(x)$. This means that the solutions are exponentially growing and decaying instead of oscillating. The WKB method works well for tunnel barriers that are either high or wide; in these cases the coefficient in front of the growing function is negligible. The wavefunction on the far side of the barrier is smaller by the amount the exponentially decreasing function falls over the width of the barrier.

The tunneling probability is given by the ratio of incident and emitted probability flux. Since this is given by the *square* of the wavefunction, we have a WKB tunneling probability of

$$T^{WKB} = e^{-2\gamma}, \tag{42}$$

where

$$\gamma = \frac{1}{\hbar}\int_a^b p(x)dx. \tag{43}$$

The integration bounds a and b are the bounds of the barrier.

Our only task is to determine the form of $p(x)$ and do the integration to find γ. For the planar approximation, the applied bias voltage drops evenly across the entire vacuum gap; the barrier is a trapezoid. We have, then,

$$\gamma = \frac{1}{\hbar}\int_0^d \sqrt{2m(-\frac{eV}{d_{gap}}x + E_F + \phi - E_z)}dx \tag{44}$$

where d is the barrier width, V is the applied bias voltage, and ϕ is the barrier height above the Fermi energy. In this planar approximation, Ez is the energy determined by the 1-dimensional perpendicular component of the momentum, $\frac{\hbar^2 k_z^2}{2m}$.

This is a trivial integral; we evaluate it to

$$\gamma = \frac{2^{3/2}m^{1/2}d}{3\hbar eV}\left((E_F + \phi - E_z)^{3/2} - (E_F + \phi - eV - E_z)^{3/2}\right). \tag{45}$$

But Simmons made a further simplification by supposing that the variation of the barrier height was small compared to the average height. Then the integral can be written as the product of the barrier thickness d times the average height. A correction factor β is included, yielding

$$T(E_z) \approx e^{\frac{-2^{3/2}m^{1/2}d}{\hbar}\beta\sqrt{E_F+\overline{\phi}-E_z}} \tag{46}$$

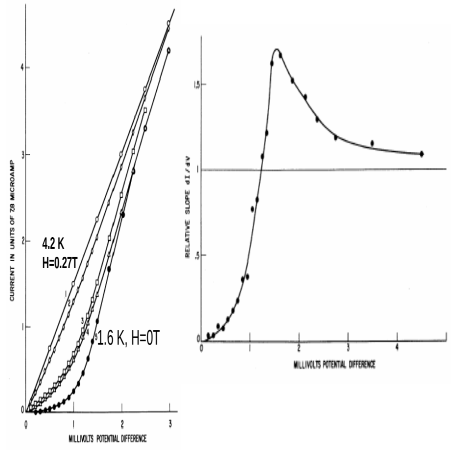
1.6 Tunnel Current

We can clearly see that

$$J = \frac{me}{2\pi^2\hbar^3}\left(eV\int_0^{E_F-eV} e^{Ad\sqrt{E_F+\overline{\phi}-E_z}}dE_z + \int_{E_F-eV}^{E_F}(E_F - E_z)e^{Ad\sqrt{E_F+\overline{\phi}-E_z}}dE_z\right) \tag{47}$$

where $A = 2\beta\sqrt{\frac{2m}{\hbar^2}}$. Performing the integral yields the Simmons tunneling formula

$$J = \frac{\alpha}{d^2}\left(\overline{\phi}e^{-Ad\sqrt{\overline{\phi}}} - (\overline{\phi} + eV)e^{-Ad\sqrt{\overline{\phi}+eV}}\right) \tag{48}$$



where $\alpha = \frac{e}{4\pi^2\beta^2\hbar}$
For $eV << \overline{\phi}$, this expression reduces to

$$J \approx \frac{\alpha}{d^2} eVe^{-Ad\sqrt{\overline{\phi}}} \tag{49}$$

Which verifies our assertion that the tunnel current is linear with voltage at small bias.

2 Normal-Superconductor tunneling

In 1960, Ivar Giaever performed the first direct measurement of the gap in density of states around the Fermi energy of a superconductor. This confirmed the BCS theory (for which Bardeen, Cooper and Schrieffer won the Nobel prize in 1972) and won Giaever his own Nobel in 1973 with Brian Josephson and Leo Esaki.

The tunnel current in this case can be written as the overlap between the density of initial (normal metal) and final (superconductor) states, and taking into account the Pauli exclusion principle:

$$I \propto \int_0^\infty N_{Normal} N_{superconductor}[f(E+eV) - f(E)]dE \tag{50}$$

Compared to the superconducting DOS, the DOS of the normal metal is slowly varying within the window defined by the term in brackets. Therefore, we can take it out of the integral:

$$\propto N_{Normal} \int_0^\infty N_{superconductor}[f(E+eV) - f(E)]dE \tag{51}$$

Now, if we take the derivative with respect to the applied voltage, we calculate the conductance:

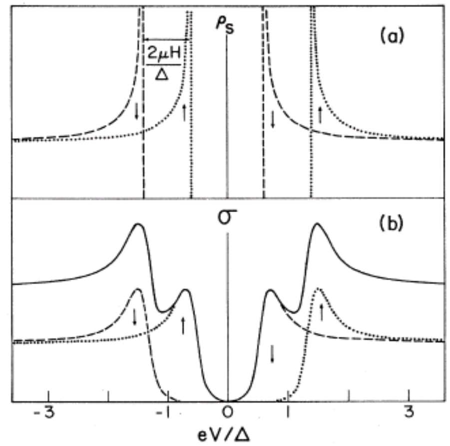
$$\frac{dI}{dV} \propto \int N_{superconductor} \frac{d[f(E+eV) - f(E)]}{dV} dE \tag{52}$$

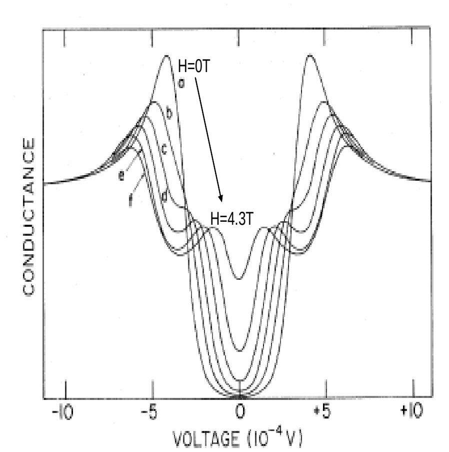
Since $\frac{f(E+eV)}{dV} = \delta(E - (E_F - eV))$,

$$\frac{dI}{dV} \propto N_{superconductor}(E_F - eV). \tag{53}$$

So we can directly determine the superconductor DOS at a given energy by scanning the applied voltage and measuring the conductance.

Giaever used Pb as the superconductor and Al as the normal metal, since it forms a self-terminating, pinhole-free oxide tunnel barrier. Measurements were made at temperatures between the critical transition temperatures (7.2K for Pb, 1.2K for Al), and compared to conductance found when an in-plane magnetic field was sufficient to destroy the superconducting state.





3 Ferromagnet-Superconductor Tunneling

Note that the BCS DOS is the sum of spin up and spin down DOS. In the early 1970s, Meservey and Tedrow performed influential measurements of ferromagnetic spin polarization with a modification of Giaever's technique. They used Al as the superconductor and applied strong in-plane fields which were not strong enough to destroy the superconducting state. This caused a Zeeman splitting of spin up and down in the superconductor, and these split states could individually probe the DOS of spin up and down in a ferromagnetic electrode. Assymetry therefore implied a polarization of tunneling electrons.

If we label the four peaks from right to left (M&T's convention) as $\sigma_1, \sigma_2, \sigma_3, \sigma_4$, the polarization

$$P = \frac{N_\uparrow - N_\downarrow}{N_\uparrow + N_\downarrow} \tag{54}$$

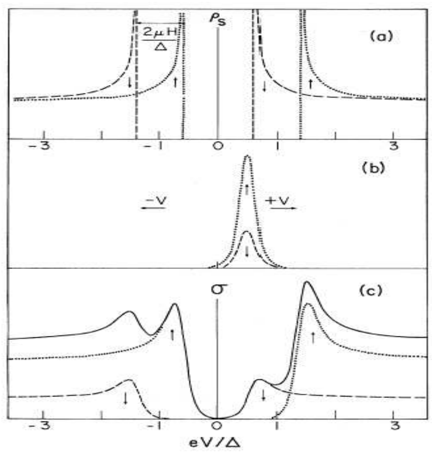
can be determined simply by noting that the spin-up density of states $N_\uparrow$ is proportional to $\sigma_4 - \sigma_2$ and the spin-up density of states $N_\uparrow$ is proportional to $\sigma_1 - \sigma_3$. Therefore we have

$$P = \frac{\sigma_4 - \sigma_2 - \sigma_1 + \sigma_3}{\sigma_4 - \sigma_2 + \sigma_1 - \sigma_3}. \tag{55}$$

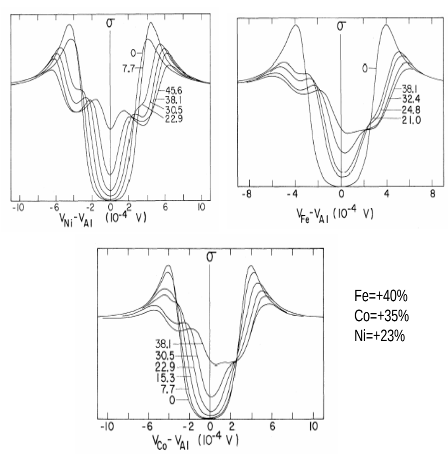
The spin polarizations of many ferromagnets were measured in this way.

4 Julliere Model

With the measurements of tunneling spin polarizations made using FM-SC tunnel junctions, Julliere in the early 1970s realized that FM-FM TJs would demonstrate magnetoresistance. He fabricated junctions using the semiconductor Ge as the tunnel barrier and found up to 14% MR at low temperatures. His model for this phenomenon took into



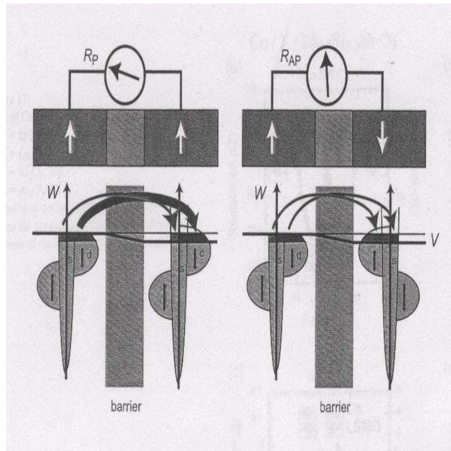
(a)
(b)
(c)
2μH/Δ
ρs
σ
-V
+V
eV/Δ



σ
V_Ni - V_Al (10^-4 V)
V_Fe - V_Al (10^-4 V)
V_Co - V_Al (10^-4 V)
Fe=+40%
Co=+35%
Ni=+23%

account only the spin polarizations of each electrode and imposed strict spin conservation across the tunnel barrier so that a spin-up electron in electrode 1 had to fill a spin-up state in electrode 2. Then,

$$\%MR = \frac{\Delta R}{R} = \frac{R_{AP} - R_P}{R_P} \tag{56}$$



The tunnel current can simply be related to the product of initial and final DOS. Since the spin-up and spin-down currents are in parallel, and $V = IR$,

$$R_{AP} \propto \frac{V}{N_1^m N_2^M + N_1^M N_2^m} \tag{57}$$

$$R_P \propto \frac{V}{N_1^m N_2^m + N_1^M N_2^M} \tag{58}$$

where in the DOS superscripts m stands for minority spin and M for majority spin.
For simplicity,

$$N_{1,2}^m = \downarrow \tag{59}$$

$$N_{1,2}^M = \uparrow \tag{60}$$

Then,

$$\frac{\Delta R}{R} = \frac{\frac{1}{\uparrow\downarrow+\downarrow\uparrow} - \frac{1}{\downarrow\downarrow+\uparrow\uparrow}}{\frac{1}{\downarrow\downarrow+\uparrow\uparrow}} = \frac{\downarrow\downarrow + \uparrow\uparrow - \uparrow\downarrow - \downarrow\uparrow}{\uparrow\downarrow + \downarrow\uparrow} \tag{61}$$

$$\frac{\Delta R}{R} = \frac{2(\uparrow - \downarrow)^2}{4\uparrow\downarrow} = \frac{2(\uparrow - \downarrow)^2}{(\uparrow + \downarrow)^2 - (\uparrow - \downarrow)^2} = \frac{2\frac{(\uparrow-\downarrow)^2}{(\uparrow+\downarrow)^2}}{\frac{(\uparrow+\downarrow)^2}{(\uparrow+\downarrow)^2} - \frac{(\uparrow-\downarrow)^2}{(\uparrow+\downarrow)^2}} = \frac{2P^2}{1 - P^2} \tag{62}$$

since the density of states asymmetry defines the spin polarization. In the case that the polarizations of the two electrodes are unequal, the result is simply generalized to

$$\frac{\Delta R}{R} = \frac{2P_1P_2}{1 - P_1P_2} \tag{63}$$

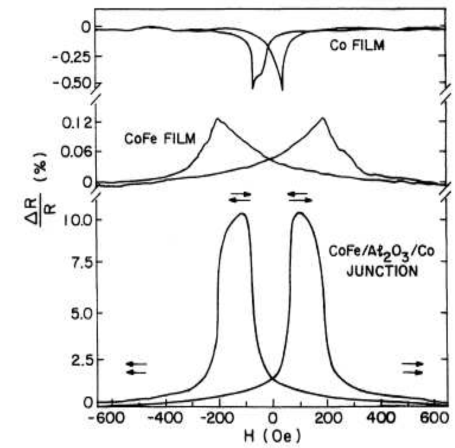


Figure 2: Moodera, PRL 74 3273 (1995)

5 Slonczewski's Theory

Julliere's formula was a first naive approach to predicting the magnetoresistance of magnetic tunnel junctions. However, it did not predict any effect of parameters other than electrode spin polarization. Slonczewski proposed a model whereby the details of the electron wavefunction in the barrier affected the predicted MR.

He approached the problem in much the same way we learn about single-barrier tunneling in undergraduate QM. However, he had to treat spin up and spin down wavefunctions separately, and the coupling of these wavefunctions across the barrier leads to a basis reformulation. Since the two FM have an angle θ between their respective magnetizations, the local definitions of "spin-up" (i.e. spin aligned parallel to the magnetization) and "spin-down" (i.e. antialigned to the magnetization) we must write

$$\Psi_{\uparrow}^{FM1} = \Psi_{\uparrow}^{FM2}\cos(\theta/2) + \Psi_{\downarrow}^{FM2}\sin(\theta/2) \tag{64}$$

$$\Psi_{\downarrow}^{FM1} = -\Psi_{\uparrow}^{FM2}\sin(\theta/2) + \Psi_{\downarrow}^{FM2}\cos(\theta/2) \tag{65}$$

where the $-$ is to make the wavefunctions orthogonal, and $\theta/2$ because the orthogonal spin-up and -down wavefunctions have an angle π between them.

Matching boundary conditions at both sides of the barrier, and then applying the particle current density expression discussed previously results in a conductance

$$G \propto 1 + P_{fb}^2\cos(\theta) \tag{66}$$

To calculate MR, we use

$$\frac{\Delta R}{R} = \frac{G(0) - G(\pi)}{G(\pi)} = \frac{1 + P_{fb}^2 - (1 - P_{fb}^2)}{1 - P_{fb}^2} = \frac{2P_{fb}^2}{1 - P_{fb}^2} \tag{67}$$

This looks like Julliere's formula, only $P \rightarrow P_{fb}$!. However, Slonczewski showed that instead of the usual definition of spin polarization

$$P = \frac{k_\uparrow - k_\downarrow}{k_\uparrow + k_\downarrow}, \tag{68}$$

his careful treatment yielded an *effective* polarization

$$P = \frac{k_\uparrow - k_\downarrow}{k_\uparrow + k_\downarrow}\frac{\kappa^2 - k_\uparrow k_\downarrow}{\kappa^2 + k_\uparrow k_\downarrow}, \tag{69}$$