

# Tunneling phenomena in solids

## Lecture 6. Tunneling in ferromagnet-insulator-ferromagnet junctions

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## Part 1: spin-dependent tunneling

## Exchange interaction in ferromagnetic metal: $s - d$ model

It is assumed that

- delocalized  $s$ -electrons provide metallic-type conductivity;
- spins of localized  $d$ -electrons are ordered parallel and form nonzero mean magnetization  $\mathbf{M}(\mathbf{r})$ ;
- spins of delocalized  $s$ -electrons interact with the mean magnetization by means of local exchange interaction.

Under these assumptions the effective Hamiltonian describing the interaction of spin of a single electron with the mean magnetization in the  $s - d$  model looks like Zeeman term

$$\hat{H}_{s-d} = -J \mathbf{m}(\mathbf{r}) \cdot \hat{\boldsymbol{\sigma}} = -J m_x(\mathbf{r}) \cdot \hat{\sigma}_x - J m_y(\mathbf{r}) \cdot \hat{\sigma}_y - J m_z(\mathbf{r}) \cdot \hat{\sigma}_z.$$

Here  $J > 0$  is a constant of exchange interaction and it has dimension of energy (Joule or eV);  $\mathbf{m}(\mathbf{r}) = \mathbf{M}(\mathbf{r})/M_s$  is unit vector parallel to the local magnetization,  $M_s$  is the saturated magnetization;  $\hat{\boldsymbol{\sigma}} = \{\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z\}$  is the operator of electron spin (i. e. vector of the Pauli matrices)

$$\hat{\sigma}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \hat{\sigma}_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \hat{\sigma}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Thus, electrons tend to align their spins along the magnetization vector  $\mathbf{m}(\mathbf{r})$ .

## Electronic waves in uniformly magnetized ferromagnet

We start with time-dependent matrix Pauli equation for two-component wave function (also known as spinor), which is natural generalization of the Schrodinger equation

$$i\hbar \frac{\partial}{\partial t} \begin{pmatrix} \Psi^{(1)} \\ \Psi^{(2)} \end{pmatrix} = \hat{H} \begin{pmatrix} \Psi^{(1)} \\ \Psi^{(2)} \end{pmatrix}, \quad \text{where} \quad \hat{H} = -\frac{\hbar^2}{2m^*} \Delta + U(\mathbf{r}) - J \mathbf{m}(\mathbf{r}) \cdot \hat{\sigma},$$

where  $\hat{H}$  is single-electron Hamiltonian. The first and the second terms correspond to kinetic and potential energies; the last term  $-J \mathbf{m}(\mathbf{r}) \cdot \hat{\sigma}$  is the effective exchange interaction in the  $s-d$  model.

We consider the stationary state with the given total energy  $E_{\parallel}$

$$\begin{pmatrix} \Psi^{(1)}(\mathbf{r}, t) \\ \Psi^{(2)}(\mathbf{r}, t) \end{pmatrix} = \begin{pmatrix} \psi^{(1)}(\mathbf{r}) \\ \psi^{(2)}(\mathbf{r}) \end{pmatrix} \cdot e^{-iE_{\parallel} t/\hbar}.$$

After substituting this function into non-stationary Pauli equation, we get matrix equation for time-independent component of the wave function

$$\hat{H} \begin{pmatrix} \psi^{(1)}(\mathbf{r}) \\ \psi^{(2)}(\mathbf{r}) \end{pmatrix} = E_{\parallel} \begin{pmatrix} \psi^{(1)}(\mathbf{r}) \\ \psi^{(2)}(\mathbf{r}) \end{pmatrix}$$

We continue with an analysis of one-dimensional scattering problem for spin-polarized electron moving along  $\xi$ -axis

$$\hat{H}_\xi = -\frac{\hbar^2}{2m^*} \frac{d^2}{d\xi^2} + U_0 - J \mathbf{m} \cdot \hat{\sigma},$$

where the orientation of the  $\xi$ -axis do not relate to the magnetization vector  $\mathbf{m}$ ,  $U_0$  is the mean potential energy, which does not depend of coordinate for uniform ferromagnet.

We introduce the cartesian coordinate system  $(x, y, z)$ , where  $z$ -axis is parallel to  $\mathbf{m}$ . This axis can be used as axis of spin quantization, then  $J \mathbf{m} \cdot \hat{\sigma}$  becomes diagonal:  $J \sigma_z$ .

Only in this case the components of the spinor can be associated with wave functions for electron with spin-up ( $\psi^{(1)} = \psi_\uparrow$ ) and for electron with spin-down ( $\psi^{(2)} = \psi_\downarrow$ ).

Inside the uniform ferromagnet the matrix Pauli equation is reduced to two independent scalar differential equations for  $\psi_\uparrow$  and  $\psi_\downarrow$

$$-\frac{\hbar^2}{2m^*} \cdot \frac{d^2 \psi_\uparrow}{d\xi^2} + U_0 \psi_\uparrow - J \psi_\uparrow = E_\parallel \psi_\uparrow \quad \text{and} \quad -\frac{\hbar^2}{2m^*} \cdot \frac{d^2 \psi_\downarrow}{d\xi^2} + U_0 \psi_\downarrow + J \psi_\downarrow = E_\parallel \psi_\downarrow.$$

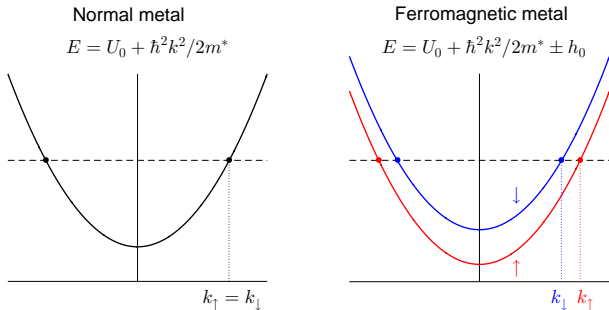
General solution of ordinary second-order differential equation is a combination of the plane waves (travelling or exponentially-decaying)

$$\psi_\uparrow = e^{\pm ik_\uparrow \xi} \quad \text{and} \quad \psi_\downarrow = e^{\pm ik_\downarrow \xi}.$$

After substituting the general solutions in the set of the independent Pauli equations, we find the dependence of the wave vectors on the energy  $E_{\parallel}$  along the  $\xi$ -axis

$$k_{\uparrow} = \sqrt{\frac{2m^*}{\hbar^2}(E_{\parallel} - U_0 + J)} \quad \text{and} \quad k_{\downarrow} = \sqrt{\frac{2m^*}{\hbar^2}(E_{\parallel} - U_0 - J)}.$$

**Intermediate conclusion:** for any  $E_{\parallel}$  value there are two spin subbands: the lower subband corresponds to electrons with spin parallel to the magnetization, while the upper subband corresponds to electrons with spin antiparallel to the magnetization:



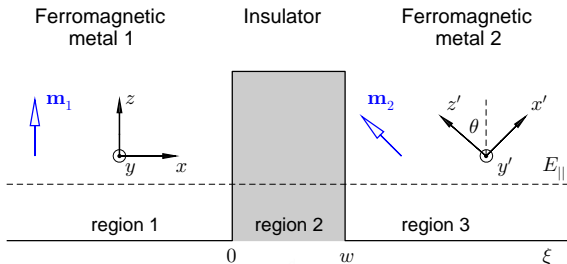
General solution for electrons in uniform ferromagnet can be written as follows

$$\psi_{\uparrow} = A_{\uparrow} e^{ik_{\uparrow}\xi} + B_{\uparrow} e^{-ik_{\uparrow}\xi} \quad \text{and} \quad \psi_{\downarrow} = A_{\downarrow} e^{ik_{\downarrow}\xi} + B_{\downarrow} e^{-ik_{\downarrow}\xi}.$$

# Tunneling in ferromagnetic junctions: formulation of problem

Slonczewski, Phys. Rev. B, vol. 39, 6995-7002 (1989).

We consider symmetric hybrid structure consisting of two bulk ferromagnetic metals with uniform distributions of magnetization ( $\mathbf{M}_1$  and  $\mathbf{M}_2$ ) separated by non-magnetic insulator. Particular orientations of  $\mathbf{M}_1$  and  $\mathbf{M}_2$  with respect to the barrier are not important – only the angle between  $\mathbf{M}_1$  and  $\mathbf{M}_2$  is of importance.



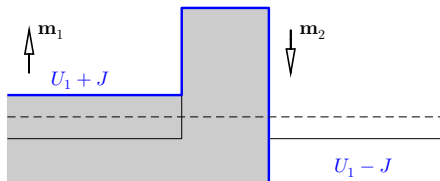
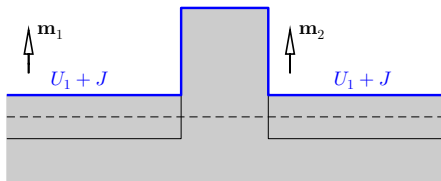
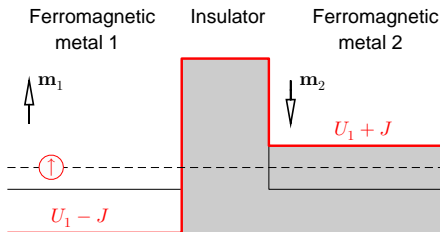
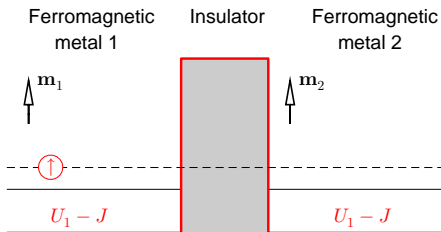
Stationary Pauli equation can be written in the form

$$\hat{H}_\xi \begin{pmatrix} \psi^{(1)} \\ \psi^{(2)} \end{pmatrix} = E_{\parallel} \begin{pmatrix} \psi^{(1)} \\ \psi^{(2)} \end{pmatrix}, \quad \text{where} \quad \hat{H}_\xi = -\frac{\hbar^2}{2m^*} \frac{d^2}{d\xi^2} + U(\xi) - J \mathbf{m} \cdot \hat{\sigma}.$$

# Qualitative explanation: spin-valve effect

parallel orientation

antiparallel orientation: no current



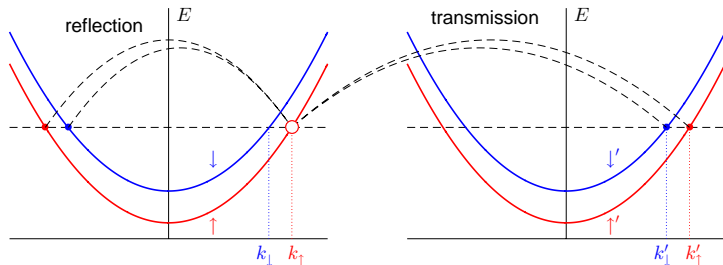


# Scattering of $\uparrow$ -electron on square potential barrier (1)

For simplicity we assume that both ferromagnetic metals have equal remanent magnetization:

$$|\mathbf{M}_1| = |\mathbf{M}_2| = M_s.$$

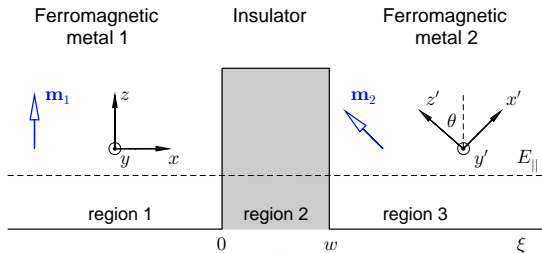
Both vectors  $\mathbf{M}_1$  and  $\mathbf{M}_2$  are generally non-parallel.



◇ Inside the metal 1 (region 1,  $\xi < 0$ ) the general solution is the superposition of the incident and two reflected waves

$$\psi_{1\uparrow} = A_{1\uparrow} e^{ik_{\uparrow}\xi} + B_{1\uparrow} e^{-ik_{\uparrow}\xi} \quad \text{and} \quad \psi_{1\downarrow} = B_{1\downarrow} e^{-ik_{\downarrow}\xi}.$$

We consider the z-axis as the axis of spin quantization: signs  $\uparrow$  and  $\downarrow$  correspond to parallel and antiparallel to both the z-axis and the vector and magnetization  $\mathbf{m}_1$ .



◊ Inside the insulating barrier (region 2,  $0 < \xi < w$ ) we can use the same  $z$ -axis for spin quantization. In this region the general solution is the superposition of exponentially decaying and increasing functions ( $E_{\parallel} < U_2$ )

$$\psi_{2\uparrow} = A_{2\uparrow} e^{-\varkappa\xi} + B_{2\uparrow} e^{\varkappa\xi} \quad \text{and} \quad \psi_{2\downarrow} = A_{2\downarrow} e^{-\varkappa\xi} + B_{2\downarrow} e^{\varkappa\xi}.$$

where  $\varkappa = \sqrt{2m^*(U_2 - E_{\parallel})}/\hbar$  is the imaginary part of the spin-independent wave vector.

◊ Inside the metal 2 (region 3,  $\xi > w$ ) we can choose the  $z'$ -axis (parallel to the local magnetization) for spin quantization, therefore the general solution due to causality principle is a combination of outgoing waves running to the right

$$\psi'_{3\uparrow} = A_{3\uparrow} e^{ik_{\uparrow}(\xi-w)} \quad \text{and} \quad \psi'_{3\downarrow} = A_{3\downarrow} e^{ik_{\downarrow}(\xi-w)}.$$

## Density of spin-polarized current: general expression

Let  $e = -|e|$  be the elementary charge, then the local electric charge is equal to

$$Q = e \sum_{\sigma} \psi_{\sigma} \psi_{\sigma}^* = e \psi_{\uparrow} \psi_{\uparrow}^* + e \psi_{\downarrow} \psi_{\downarrow}^*.$$

We use time-dependent Pauli equations and calculate the rate of local charge variations

$$\begin{aligned} \frac{\partial Q}{\partial t} &= e \frac{\psi_{\uparrow}^*}{i\hbar} \left( i\hbar \frac{\partial \psi_{\uparrow}}{\partial t} \right) + e \frac{\psi_{\uparrow}}{i\hbar} \left( i\hbar \frac{\partial \psi_{\uparrow}^*}{\partial t} \right) + e \frac{\psi_{\downarrow}^*}{i\hbar} \left( i\hbar \frac{\partial \psi_{\downarrow}}{\partial t} \right) + e \frac{\psi_{\downarrow}}{i\hbar} \left( i\hbar \frac{\partial \psi_{\downarrow}^*}{\partial t} \right) = \\ &= \frac{e}{i\hbar} \left( -\frac{\hbar^2}{2m^*} \right) \left\{ \psi_{\uparrow}^* \nabla^2 \psi_{\uparrow} - \psi_{\uparrow} \nabla^2 \psi_{\uparrow}^* + \psi_{\downarrow}^* \nabla^2 \psi_{\downarrow} - \psi_{\downarrow} \nabla^2 \psi_{\downarrow}^* \right\}. \end{aligned}$$

It can be reduced to the following form

$$\frac{\partial Q}{\partial t} + \operatorname{div} \mathbf{j} = 0, \quad \text{где} \quad \mathbf{j} = \left( \frac{e\hbar}{m^*} \right) \left\{ \operatorname{Im} \left( \psi_{\uparrow}^* \nabla \psi_{\uparrow} \right) + \operatorname{Im} \left( \psi_{\downarrow}^* \nabla \psi_{\downarrow} \right) \right\}.$$

Reminder:  $z - z^* = (a + ib) - (a - ib) = 2i \operatorname{Im} z$

For planar layered system the current density does not depend on the coordinate  $\xi$ . To calculate the tunnel current density, we will consider region 3 behind the barrier, since there are only two types of electron waves, and not three or four (as in regions 1 and 2).

## Rotation of the axis of spin quantization

To matching wave functions at the left and right sides of the barrier, it is necessary to use the same quantization axis (for example,  $z$ ), therefore the components of the wave function in the region 3 should be modified using standard formulas for spinor transformation.

Reminder: the connection between the spinor components when the spin quantization axis rotates around the  $x$ ,  $y$  and  $z$  axes respectively, is given by the following matrix relation

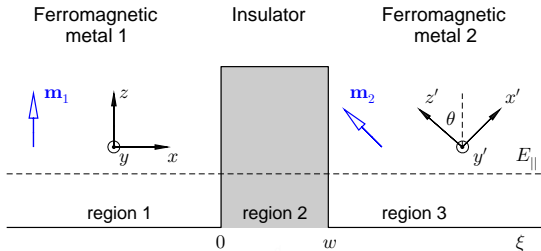
$$\begin{pmatrix} \psi^{(1)} \\ \psi^{(2)} \end{pmatrix} = \hat{S} \begin{pmatrix} \psi^{(1),'} \\ \psi^{(2),'} \end{pmatrix},$$

where

$$\hat{S}_x = \begin{pmatrix} \cos \varphi/2 & i \sin \varphi/2 \\ i \sin \varphi/2 & \cos \varphi/2 \end{pmatrix}, \quad \hat{S}_y = \begin{pmatrix} \cos \varphi/2 & \sin \varphi/2 \\ -\sin \varphi/2 & \cos \varphi/2 \end{pmatrix}, \quad \text{and}$$
$$\hat{S}_z = \begin{pmatrix} e^{i\varphi/2} & 0 \\ 0 & e^{-i\varphi/2} \end{pmatrix},$$

$\varphi$  is the rotation angle between  $z$  and  $z'$  axes.

Landau and Lifshits, *Quantum mechanics. Non-relativistic theory*



In our case, the coordinate system  $(x', y', z')$  is rotated by an angle  $\alpha$  around the  $y$  axis relative to the system  $(x, y, z)$ , therefore, to determine the components of the wave function in the  $(x, y, z)$  axes in metal 2, we have to use the rotation matrix

$$\hat{S}_y = \begin{pmatrix} \cos \alpha/2 & \sin \alpha/2 \\ -\sin \alpha/2 & \cos \alpha/2 \end{pmatrix}, \quad \text{where } \alpha = \arccos(\mathbf{m}_1 \cdot \mathbf{m}_2).$$

Thus, we come to the following expressions

$$\psi_{3\uparrow} = \psi'_{3\uparrow} \cos \frac{\alpha}{2} + \psi'_{3\downarrow} \sin \frac{\alpha}{2} = A_{3\uparrow} e^{ik_{\uparrow}(\xi-w)} \cos \frac{\alpha}{2} + A_{3\downarrow} e^{ik_{\downarrow}(\xi-w)} \sin \frac{\alpha}{2},$$

$$\psi_{3\downarrow} = -\psi'_{3\uparrow} \sin \frac{\alpha}{2} + \psi'_{3\downarrow} \cos \frac{\alpha}{2} = -A_{3\uparrow} e^{ik_{\uparrow}(\xi-w)} \sin \frac{\alpha}{2} + A_{3\downarrow} e^{ik_{\downarrow}(\xi-w)} \cos \frac{\alpha}{2}.$$

For  $\alpha \neq 0$  and  $\pi$  the spin-up and spin-down components become mixed.

## Scattering of $\uparrow$ -electron on square potential barrier (2)

In order to determine the amplitude of all waves we need to apply boundary conditions – the requirements of the continuity of the components of the spinors and their first derivatives at the left and right edges of the barrier:

$$\xi = 0: \quad A_{1\uparrow} + B_{1\uparrow} = A_{2\uparrow} + B_{2\uparrow}, \quad ik_{\uparrow} A_{1\uparrow} - ik_{\uparrow} B_{1\uparrow} = -\varkappa A_{2\uparrow} + \varkappa B_{2\uparrow}, \\ B_{1\downarrow} = A_{2\downarrow} + B_{2\downarrow}, \quad -ik_{\downarrow} B_{1\downarrow} = -\varkappa A_{2\downarrow} + \varkappa B_{2\downarrow}$$

$$\xi = w: \quad A_{2\uparrow} e^{-\varkappa w} + B_{2\uparrow} e^{\varkappa w} = A_{3\uparrow} \cos \frac{\alpha}{2} + A_{3\downarrow} \sin \frac{\alpha}{2}, \\ -\varkappa A_{2\uparrow} e^{-\varkappa w} + \varkappa B_{2\uparrow} e^{\varkappa w} = ik_{\uparrow} A_{3\uparrow} \cos \frac{\alpha}{2} + ik_{\downarrow} A_{3\downarrow} \sin \frac{\alpha}{2}, \\ A_{2\downarrow} e^{-\varkappa w} + B_{2\downarrow} e^{\varkappa w} = -A_{3\uparrow} \sin \frac{\alpha}{2} + A_{3\downarrow} \cos \frac{\alpha}{2}, \\ -\varkappa A_{2\downarrow} e^{-\varkappa w} + \varkappa B_{2\downarrow} e^{\varkappa w} = -ik_{\uparrow} A_{3\uparrow} \sin \frac{\alpha}{2} + ik_{\downarrow} A_{3\downarrow} \cos \frac{\alpha}{2}.$$

We get a system of 8 linear equations with 8 unknowns ( $B_{1\uparrow}$ ,  $B_{1\downarrow}$ ,  $A_{2\uparrow}$ ,  $A_{2\downarrow}$ ,  $B_{2\uparrow}$ ,  $B_{2\downarrow}$ ,  $A_{3\uparrow}$  и  $A_{3\downarrow}$ ) for the given amplitude of the incident wave  $A_{1\uparrow}$ .

## Solution of scattering problem for $\uparrow$ -electron

Coefficients  $B_{1\uparrow}$ ,  $B_{1\downarrow}$ ,  $A_{2\uparrow}$  and  $A_{2\downarrow}$  can be expressed through the amplitude of the incident wave  $A_{1\uparrow}$  and the coefficients  $B_{2\uparrow}$ ,  $B_{2\downarrow}$

$$B_{1\uparrow} = A_{2\uparrow} + B_{2\uparrow} - A_{1\uparrow}, \quad B_{1\downarrow} = A_{2\downarrow} + B_{2\downarrow},$$
$$A_{2\uparrow} = -\frac{2ik_{\uparrow}}{(\varkappa - ik_{\uparrow})} a_{1\uparrow} + \frac{(\varkappa + ik_{\uparrow})}{(\varkappa - ik_{\uparrow})} B_{2\uparrow}, \quad \text{and} \quad A_{2\downarrow} = \frac{(\varkappa + ik_{\downarrow})}{(\varkappa - ik_{\downarrow})} B_{2\downarrow}$$

For low-transmission barrier ( $e^{\varkappa w} \gg e^{-\varkappa w}$ ) we get the coefficients for the wave functions inside the barrier

$$B_{2\uparrow} \simeq -\frac{2ik_{\uparrow} e^{-2\varkappa w} [\varkappa^2 + k_{\uparrow}k_{\downarrow} + i\varkappa(k_{\uparrow} - k_{\downarrow}) \cos \alpha]}{(\varkappa - ik_{\uparrow})^2(\varkappa - ik_{\downarrow})} A_{1\uparrow},$$

$$B_{2\downarrow} \simeq \frac{2\varkappa k_{\uparrow} e^{-2\varkappa w} (k_{\downarrow} - k_{\uparrow}) \sin \alpha}{(\varkappa - ik_{\uparrow})^2(\varkappa - ik_{\downarrow})} A_{1\uparrow},$$

and behind the barrier

$$A_{3\uparrow} \simeq -\frac{4ik_{\uparrow}\varkappa e^{-\varkappa w}}{(\varkappa - ik_{\uparrow})^2} \cdot \cos \frac{\alpha}{2} \cdot A_{1\uparrow} \quad \text{and} \quad A_{3\downarrow} \simeq -\frac{4ik_{\uparrow}\varkappa e^{-\varkappa w}}{(\varkappa - ik_{\uparrow})(\varkappa - ik_{\downarrow})} \cdot \sin \frac{\alpha}{2} \cdot A_{1\uparrow}.$$

For non-parallel configuration ( $\alpha \neq 0$  and  $\pi$ )  $\uparrow$ - and  $\downarrow$ -components becomes interacting.

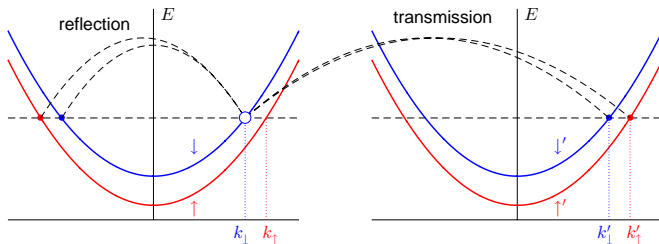
## Scattering of $\downarrow$ -electron on square potential barrier

Now consider the scattering of a spin-down particle in a similar system. The general solution in all three areas should have the following form

$$\psi_{1\uparrow} = B_{1\uparrow} e^{-ik_{\uparrow}\xi}, \quad \psi_{1\downarrow} = A_{1\downarrow} e^{ik_{\downarrow}\xi} + B_{1\downarrow} e^{-ik_{\downarrow}\xi}.$$

$$\psi_{2\uparrow} = A_{2\uparrow} e^{-\alpha\xi} + B_{2\uparrow} e^{\alpha\xi}, \quad \psi_{2\downarrow} = A_{2\downarrow} e^{-\alpha\xi} + B_{2\downarrow} e^{\alpha\xi}.$$

$$\psi'_{3\uparrow} = A_{3\uparrow} e^{ik'_{\uparrow}(\xi-w)}, \quad \psi'_{3\downarrow} = A_{3\downarrow} e^{ik'_{\downarrow}(\xi-w)}.$$





The conditions for the continuity of the components of the spinors and their first derivatives of the left and right edges of the barrier have the following form

$$\xi = 0 : \quad B_{1\uparrow} = A_{2\uparrow} + B_{2\uparrow}, \quad -ik_{\uparrow} B_{1\uparrow} = -\varkappa A_{2\uparrow} + \varkappa B_{2\uparrow}, \\ A_{1\downarrow} + B_{1\downarrow} = A_{2\downarrow} + B_{2\downarrow}, \quad ik_{\downarrow} A_{1\downarrow} - ik_{\downarrow} B_{1\downarrow} = -\varkappa A_{2\downarrow} + \varkappa B_{2\downarrow},$$

$$\xi = w : \quad A_{2\uparrow} e^{-\varkappa w} + B_{2\uparrow} e^{\varkappa w} = A_{3\uparrow} \cos \frac{\alpha}{2} + A_{3\downarrow} \sin \frac{\alpha}{2}, \\ -\varkappa A_{2\uparrow} e^{-\varkappa w} + \varkappa B_{2\uparrow} e^{\varkappa w} = ik_{\uparrow} A_{3\uparrow} \cos \frac{\alpha}{2} + ik_{\downarrow} A_{3\downarrow} \sin \frac{\alpha}{2}, \\ A_{2\downarrow} e^{-\varkappa w} + B_{2\downarrow} e^{\varkappa w} = -A_{3\uparrow} \sin \frac{\alpha}{2} + A_{3\downarrow} \cos \frac{\alpha}{2}, \\ -\varkappa A_{2\downarrow} e^{-\varkappa w} + \varkappa B_{2\downarrow} e^{\varkappa w} = -ik_{\uparrow} A_{3\uparrow} \sin \frac{\alpha}{2} + ik_{\downarrow} A_{3\downarrow} \cos \frac{\alpha}{2}.$$

For low-transmission barrier ( $e^{\varkappa w} \gg e^{-\varkappa w}$ ) we get the coefficients for the wave functions behind the barrier

$$A_{3\uparrow} \simeq \frac{4i\varkappa k_{\downarrow} e^{-\varkappa w}}{(\varkappa - ik_{\downarrow})(\varkappa - ik_{\uparrow})} \cdot \sin \frac{\alpha}{2} \cdot A_{1\downarrow} \quad \text{and} \quad A_{3\downarrow} \simeq -\frac{4i\varkappa k_{\downarrow} e^{-\varkappa w}}{(\varkappa - ik_{\downarrow})^2} \cdot \cos \frac{\alpha}{2} \cdot A_{1\downarrow}.$$

For non-parallel configuration ( $\alpha \neq 0$  and  $\pi$ )  $\uparrow -$  and  $\downarrow -$  components becomes interacting.

## Density of spin-polarized current behind the barrier

We have shown that the incident spin-polarized particles induces the following spin-polarized components in a right-handed ferromagnetic metal ( $\xi > w$ )

$$\psi'_{\uparrow} = A_{3\uparrow} e^{ik_{\uparrow}(\xi-w)}, \quad \psi'_{\downarrow} = A_{3\downarrow} e^{ik_{\downarrow}(\xi-w)}.$$

This corresponds to the  $\xi$ -component of the tunneling current density

$$\begin{aligned} j &= \left( \frac{e\hbar}{m^*} \right) \left\{ \text{Im} (A_{3\uparrow}^* (ik_{\uparrow}) A_{3\uparrow}) + \text{Im} (A_{3\downarrow}^* (ik_{\downarrow}) A_{3\downarrow}) \right\} = \\ &= \left( \frac{e\hbar}{m^*} \right) \left\{ k_{\uparrow} |A_{3\uparrow}|^2 + (\text{Re } k_{\downarrow}) |A_{3\downarrow}|^2 \right\}. \end{aligned}$$

1. When  $\uparrow$ -electron is scattered, the wave amplitudes in the region behind the barrier are determined by the relations

$$A_{3\uparrow} \simeq -\frac{4ik_{\uparrow}\chi e^{-\chi w}}{(\chi - ik_{\uparrow})^2} \cdot \cos \frac{\alpha}{2} \cdot A_{1\uparrow} \quad \text{and} \quad A_{3\downarrow} \simeq -\frac{4ik_{\uparrow}\chi e^{-\chi w}}{(\chi - ik_{\uparrow})(\chi - ik_{\downarrow})} \cdot \sin \frac{\alpha}{2} \cdot A_{1\uparrow}.$$

This corresponds to an electric current density equal to

$$j_{\uparrow} = e \left( \frac{\hbar k_{\uparrow}}{m^*} |A_{1\uparrow}|^2 \right) \cdot \frac{16 k_{\uparrow} \chi^2 k_{\uparrow} e^{-2\chi w}}{(\chi^2 + k_{\uparrow}^2)(\chi^2 + k_{\downarrow}^2)} \cdot \left\{ \left( \cos \frac{\alpha}{2} \right)^2 + \frac{(\text{Re } k_{\downarrow})}{k_{\uparrow}} \frac{(\chi^2 + k_{\uparrow}^2)}{(\chi^2 + k_{\downarrow}^2)} \left( \sin \frac{\alpha}{2} \right)^2 \right\}.$$

2. When  $\downarrow$ -electron is scattered, the wave amplitudes in the region behind the barrier are determined by the relations

$$A_{3\uparrow} \simeq + \frac{4i\chi k_{\downarrow} e^{-\chi w}}{(\chi - ik_{\downarrow})(\chi - ik_{\uparrow})} \cdot \sin \frac{\alpha}{2} \cdot A_{1\downarrow} \quad \text{and} \quad A_{3\downarrow} \simeq - \frac{4i\chi k_{\downarrow} e^{-\chi w}}{(\chi - ik_{\downarrow})^2} \cdot \cos \frac{\alpha}{2} \cdot A_{1\downarrow}.$$

This corresponds to an electric current density equal to

$$j_{\downarrow} = e \left( \frac{\hbar k_{\downarrow}}{m^*} |A_{1\downarrow}|^2 \right) \cdot \frac{16k_{\downarrow}\chi^2 k_{\downarrow} e^{-2\chi w}}{(\chi^2 + k_{\downarrow}^2)(\chi^2 + k_{\uparrow}^2)} \cdot \left\{ \frac{k_{\uparrow}(\chi^2 + k_{\downarrow}^2)}{k_{\downarrow}(\chi^2 + k_{\uparrow}^2)} \left( \sin \frac{\alpha}{2} \right)^2 + \left( \cos \frac{\alpha}{2} \right)^2 \right\}.$$

3. Let us define the transmission coefficients as the ratio of the current density to the probability flux of the incident particle

$$\mathcal{T}_{\uparrow} = \frac{16k_{\uparrow}\chi^2 k_{\uparrow} e^{-2\chi w}}{(\chi^2 + k_{\uparrow}^2)(\chi^2 + k_{\downarrow}^2)} \cdot \left\{ \left( \cos \frac{\alpha}{2} \right)^2 + \frac{(\text{Re } k_{\downarrow})}{k_{\uparrow}} \frac{(\chi^2 + k_{\uparrow}^2)}{(\chi^2 + k_{\downarrow}^2)} \left( \sin \frac{\alpha}{2} \right)^2 \right\},$$

$$\mathcal{T}_{\downarrow} = \frac{16k_{\downarrow}\chi^2 k_{\downarrow} e^{-2\chi w}}{(\chi^2 + k_{\downarrow}^2)(\chi^2 + k_{\uparrow}^2)} \cdot \left\{ \frac{k_{\uparrow}(\chi^2 + k_{\downarrow}^2)}{k_{\downarrow}(\chi^2 + k_{\uparrow}^2)} \left( \sin \frac{\alpha}{2} \right)^2 + \left( \cos \frac{\alpha}{2} \right)^2 \right\}.$$

Compare these expressions with the transmission of non-magnetic barrier (see lecture 1)

## Part 2: tunneling magnetoresistance and spin-polarized STM

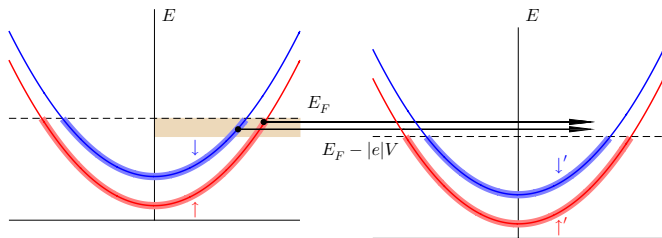
## Tunneling conductance: case of low bias and low temperature

For simplicity, we will assume that ferromagnetic metals are the same with equal effective masses, Fermi energies, work function and magnetization.

Let us consider electrons located in ferromagnetic metal 1 (emitter) in a narrow energy band from  $E_F - \delta E$  to  $E_F$  (where  $\delta E = |e \delta V|$ ). Such electrons will tunnel with almost the same probability and create the current in ferromagnetic metal 2 (collector) equal to

$$\delta I = \text{const} \cdot \{T_{\uparrow} + T_{\downarrow}\}_{E=E_F} \cdot \delta V \implies G = \left( \frac{\delta I}{\delta V} \right)_{V \rightarrow 0} = \text{const} \cdot \{T_{\uparrow} + T_{\downarrow}\}_{E=E_F},$$

where the numerical coefficient takes into account the contribution of geometric factors, the shape of barriers and density of states near  $E_F$ .



In the general case, both spin subbands can be occupied and, therefore, we need to take into account the contributions of incident particles with spin up and spin down

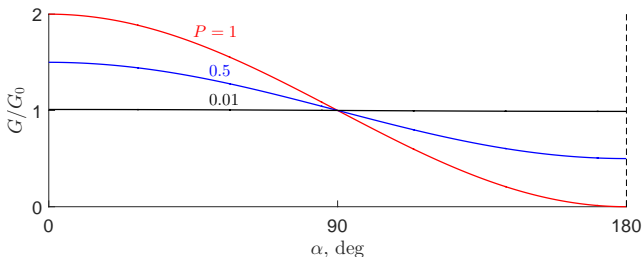
$$G = \text{const} \cdot \left\{ T_{\uparrow} + T_{\downarrow} \right\}_{E=E_F} =$$

$$= \text{const} \cdot 16\chi^2 e^{-2\chi w} \frac{(\chi^2 + k_{\uparrow}k_{\downarrow})^2 (k_{\uparrow} + k_{\downarrow})^2}{(\chi^2 + k_{\uparrow}^2)^2 (\chi^2 + k_{\downarrow}^2)^2} \cdot \left\{ 1 + \frac{(\chi^2 - k_{\uparrow}k_{\downarrow})^2 (k_{\uparrow} - k_{\downarrow})^2}{(\chi^2 + k_{\uparrow}k_{\downarrow})^2 (k_{\uparrow} + k_{\downarrow})^2} \cos \alpha \right\}.$$

We introduce the effective spin polarization

$$P = \frac{(k_{\uparrow} - k_{\downarrow})(\chi^2 - k_{\uparrow}k_{\downarrow})}{(k_{\uparrow} + k_{\downarrow})(\chi^2 + k_{\uparrow}k_{\downarrow})} \quad \text{and} \quad |P| < 1.$$

**Important conclusion:** the tunneling current for given tunneling voltage depends on the mutual orientation of the magnetization vectors as  $1 + P^2 \cos \alpha$



# Resulting tunneling conductance: summation over all modes

Slonczewski, Phys. Rev. B, vol. 39, 6995-7002 (1989).

If we take into account all numerical factors, then

– the case of single occupied sub-band:

$$G = \frac{\varkappa}{\hbar w} \left[ \frac{|e|}{\pi} \frac{\varkappa k_{\uparrow} e^{-\varkappa w}}{(\varkappa^2 + k_{\uparrow}^2)} \right]_{E=E_F}^2 \cdot (1 + \cos \alpha);$$

– the case of two occupied sub-bands:

$$G = \frac{\varkappa}{\hbar w} \left[ \frac{|e| \varkappa (\varkappa^2 + k_{\uparrow} k_{\downarrow}) (k_{\uparrow} + k_{\downarrow}) e^{-\varkappa w}}{\pi (\varkappa^2 + k_{\downarrow}^2) (\varkappa^2 + k_{\uparrow}^2)} \right]_{E=E_F}^2 \cdot (1 + P^2 \cos \alpha),$$

where  $P = \frac{(k_{\uparrow} - k_{\downarrow})(\varkappa^2 - k_{\uparrow} k_{\downarrow})}{(k_{\uparrow} + k_{\downarrow})(\varkappa^2 + k_{\uparrow} k_{\downarrow})}$  is the effective spin polarization

# Spin-polarized scanning tunneling spectroscopy

Spin-dependent tunneling and tunneling magnetoresistance (TMR):  $\Delta G/G_0 \simeq 14\%$

## TUNNELING BETWEEN FERROMAGNETIC FILMS

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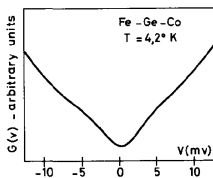


Fig. 1. Conductance versus voltage of Fe-Ge-Co junctions at 4.2K. Ge layer width is about 100 Å.

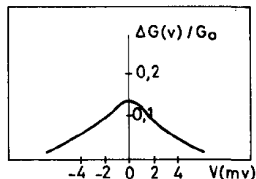


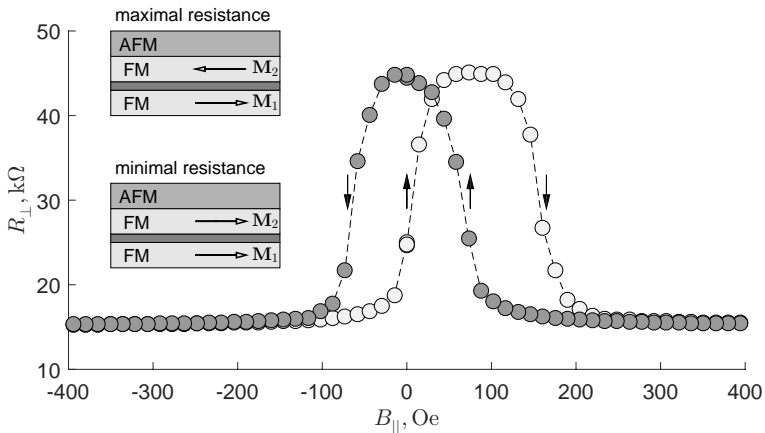
Fig. 2. Relative conductance  $(\Delta G/G)_{V=0}$  of Fe-Ge-Co junctions at 4.2K.  $\Delta G$  is the difference between the two conductance values corresponding to parallel and antiparallel magnetizations of the two ferromagnetic films.

Julliere, Phys. Lett. A, vol. 54, 225-226 (1975).



# Tunneling magnetoresistive element

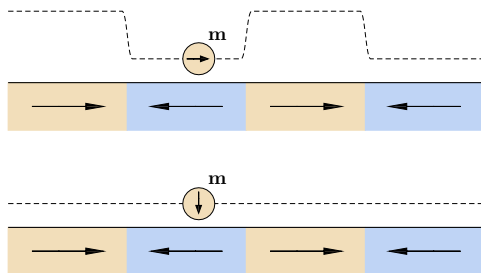
Pashen'kin, Sapozhnikov, Gusev *et al.* Magnetoelectric Effect in CoFeB/MgO/CoFeB Magnetic Tunnel Junctions // JETP Letters, v. 111, 690-693 (2020)



# Spin-polarized scanning tunneling spectroscopy: an idea

Possible modes of operation:

1. Tunneling microscopy in the regimes of given current or given height:  $z(x, y) \rightarrow M(x, y)$
2. Scanning tunneling spectroscopy:  $z(x, y)$  and  $dI/dV(x, y) \rightarrow M(x, y)$
3. Modulation technique:  $z(x, y) + m(t) \rightarrow M(x, y)$



# Spin-polarized scanning tunneling spectroscopy: imaging of terraces with different magnetization

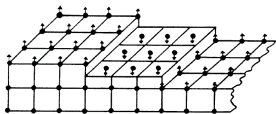


FIG. 1. Topological antiferromagnetic order of the Cr(001) surface with terraces separated by monatomic steps. Different terraces are magnetized in opposite directions. Only surface spins are indicated. (Figure taken from Ref. 7.)

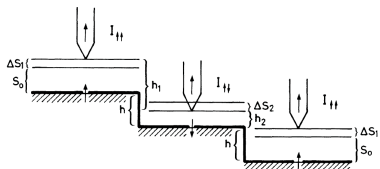
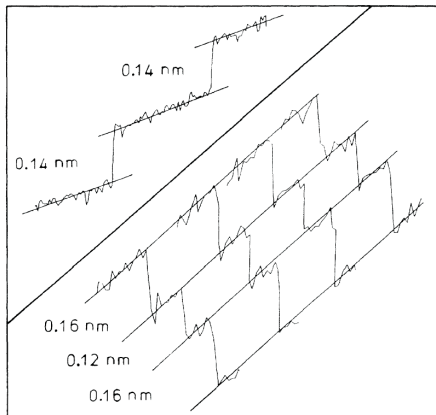


FIG. 4. Schematic drawing of a ferromagnetic tip scanning over alternately magnetized terraces separated by monatomic steps of height  $h$ . An additional contribution from SP tunneling leads to alternating step heights  $h_1 = h + \Delta S_1 + \Delta S_2$  and  $h_2 = h - \Delta S_1 - \Delta S_2$ .



Wiesendanger, Güntherodt, Güntherodt, Gambino, Ruf. Phys. Rev. Lett., vol. 111, 247-250 (1990)

# Spin-polarized scanning tunneling spectroscopy: imaging of ferromagnetic domains

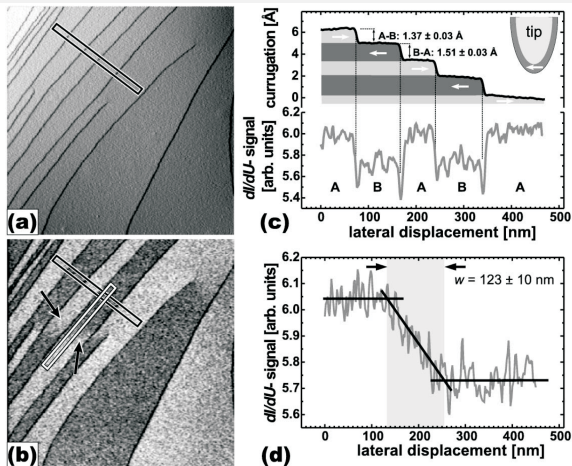


FIG. 2. (a) Large scale constant-current STM image ( $1 \mu\text{m} \times 1 \mu\text{m}$ ) of the Cr (001) surface showing many terraces separated by monatomic steps. Three screw dislocations are visible. The data were again obtained with a Fe-coated probe tip using a tunneling current  $I = 0.18$  nA and a sample bias  $U = -60$  mV. (b) Spin-polarized spectroscopic image of the same surface region as shown in (a). Again, the measured  $dI/dU$  signal at the surface state peak position changes between two levels whenever a monatomic step of the Cr(001) surface is crossed. However, an additional change can now be observed within (001) terraces in the surroundings of screw dislocations (see arrows). This is caused by spin frustration effects in the vicinity of such screw dislocations. (c) The top part

Kleiber, Bode, Ravlić, Wiesendanger. Phys. Rev. Lett., vol. 85, 4606-4609 (2000)

# Spin-polarized scanning tunneling spectroscopy: imaging of ferromagnetic nanoparticles

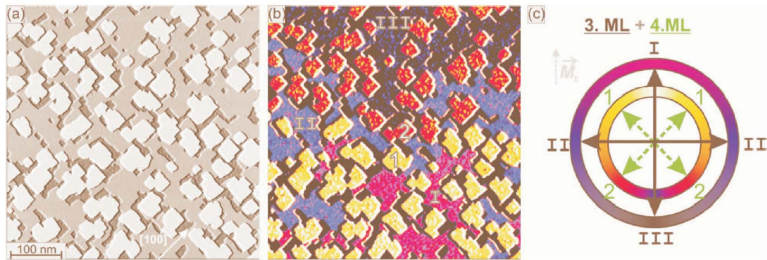


FIG. 20. (Color) Thin film of 3.2 ML Fe on W(001) grown at a temperature  $T \sim 525$  K. (a) Constant-current STM topograph showing that patches of 2, 3, and 4 ML Fe on W(001) are exposed at the surface. (b) Simultaneously measured spin-resolved  $dI/dU$  map showing three magnetic contrast levels (I–III) on the third monolayer and two magnetic contrast levels (1, 2) on the fourth monolayer. The derived magnetization axes for the third and fourth monolayers are sketched in (c). From von Bergmann, Bode, and Wiesendanger, 2004.

von Bergmann, Bode, and Wiesendanger, J. Magn. Magn. Mater. vol. 305, 279 (2006)

# Spin-polarized scanning tunneling spectroscopy: imaging of single magnetic atoms

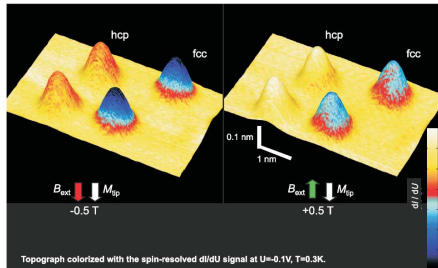


FIG. 54. (Color) SP-STM images of four Co adatoms on Pt(111) obtained with a parallel (left) or antiparallel (right) alignment of the magnetic moments of tip apex atom and Co adatoms. In this case, a sample bias voltage of  $-0.1 \text{ V}$  was chosen for which the electronic contrast, arising from the two inequivalent Co adsorption sites (fcc and hcp), is much stronger than the magnetic contrast arising from the different orientation of the Co moments in the left and in the right image. From Meier *et al.*, 2008.

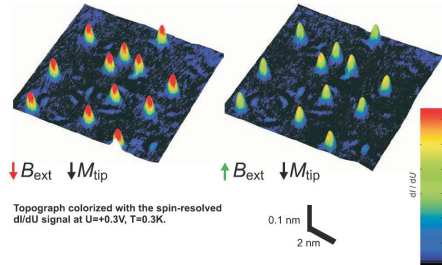


FIG. 55. (Color) Set of two SP-STM images showing several Co adatoms on Pt(111) with their spins aligned either parallel (left) or antiparallel (right) with respect to the spin orientation of the tip apex atom. In this case, a sample bias voltage of  $+0.3 \text{ V}$  was chosen for which the observed contrast difference between the left and the right image is primarily dominated by the different magnetic states of the Co adatoms, while the inequivalent Co adsorption sites cannot be distinguished. From Meier *et al.*, 2008.

Meier, Zhou, Wiebe, Wiesendanger, Science, vol. 320, 82–86 (2008)