

## Quantum basis of the spin manipulation by electric fields

**Coriolan TIUSAN** 

Department of Physics and Chemistry, Center of Superconductivity, Spintronics and Surface Science, Technical University of Cluj-Napoca, Romania and National center of Scientific Research (CNRS), France

#### Ideea: Datta and Das Transistor

S. Datta and B. Das (1990) *"Electronic analog of the electro-optic modulator*" Applied Physics Letters 56 (7): 665–667. (1990)

(1)



(2)



- Gate potential controls the source-drain current
- Used as modulator, amplifier, switch

- □ Source and drain = FM materials
- □ Conducton channel = 2DEG
- The gate electric field moduletes the electron spin state
- □ No external magnetic field

### Take advantage of the electron spin as a new degree of freedom to generate new functionalities and devices

Basic ideea: Magnetic materials can be used as Polarizer and Analyzer of electrons (spin filters)



# Spin FET



#### Photoemission/Angle-resolved photoemission spectroscopy (ARPES)

![](_page_4_Figure_1.jpeg)

-based on photoelectric effect (X, UV) => XPS, UPS

- direct experimental technique to observe the distribution of the electrons in the reciprocal space of solids = E(k) for occupied valence states

![](_page_5_Figure_0.jpeg)

Electron energy analyzers in ARPES use 2D CCD detector allowing to get the E(k) of the valence band states in a wide range of emission angles theta in one shot (at a fixed angle beta). The emission angle theta can be used for the calculation of wave vector component k, of electron in solid. A rotation of the sample by angle beta produces the 3D data set of experimental photoemission intensity,  $I(E_{kin}, k_x, k_y)$ , where  $E_{kin}$  is the kinetic energy of electron and  $k_v$  is the second in-plane component of the wave-vector calculated from the experimental geometry. In the case of spinresolved ARPES experiments the 2D CCD detector is replaced by a spindetector (e.g. classical Mott). This allows an effective separation of the spin-polarized electron beam into two channels: spin-up and spindown electrons

#### Photoemission

![](_page_6_Figure_1.jpeg)

Electron photoemission experiments on a 2D electron (Shockley) state on Au(111) surface –*G. Nicolay, F. Reinert, S. Hufner, P. Blaha, Phys. Rev. B 65 (2002)* 033407 respectiv *F. Reinert, G. Nicolay, S. Schmidt, D. Ehm, S. Hufner, Phys. Rev. B 63 (2001) 115415.* The experimens are taken at 30K. Bottom panel: the band structure  $E(k_x)$  along the  $\overline{\Gamma M}$  direction.

Middle panel: cut on  $(k_x, k_y)$  representation (top panel) at  $k_y = 0$ 

#### Measuring $\Delta k \Rightarrow$ Rashba constant $\alpha$

 $\Box$   $\alpha_R$  from ARPES for materials with important potential in spin-orbitronics (when materials with significant SO are used for generation of spin currents by spin-Hall effects).

![](_page_7_Figure_1.jpeg)

From A. Fert

Plan

- □ Starting from the non-relativistic Dirac Hamiltonian, written for the case of a 2D free- electron gas with a confinement direction perpendicular to the propagation direction, we deduce the Rashba Hamiltonian. This strategy allows the direct identification of the Rashba interaction term and interaction constant alpha, as a measure of the spin-orbit interaction. One can thus understand how alpha can be controlled via the external electric field (in Datta-Das spin transistor geometry).
- □ Within the Heisenberg-Dirac formalism, we solve the stationary Schrodinger equation by diagonalising the spin-orbit Hamiltonian and find the eigenvalues and the stationary eigenfunctions.
  - Analyse the spin-orbit influence on the calculated parabolic *E(k)* band structure and discuss how the spin-orbit constant alpha can be extracted from ARPES experiments.
  - Illustrate with some examples of ARPES for materials with important potential in spinorbitronics (when materials with significant SO are used for generation of spin currents by spin-Hall effects).
- □ Furthermore, we study the time evolution, solving the time dependent Schrodinger equation. Then, by calculating average values of the spin operators Sx, Sy, Sz we can demonstrate and discuss the spin precession .

#### Problem

□ Consider the Datta@Das transitor (Fig.)

 $\Box$  (x<sub>ref</sub>, y<sub>ref</sub>, z<sub>ref</sub>) = lab referential; z<sub>ref</sub> II **E** and z<sub>ref</sub>  $\perp$  2DEG plane

![](_page_9_Figure_3.jpeg)

![](_page_9_Figure_4.jpeg)

- □ The spin precession in external electric field is related to the **spin-orbit interaction** in the 2DEG (Rashba effect)
- □ The origin of the SPIN –ORBIT interaction is relativistic
- □ An electron moving with the velocity **v** in an external field **E** will fill in its own referential an effective magnetic field perpendicular on the direction of moving :

$$\vec{B} = -\frac{\vec{v} \times \vec{E}}{c^2}$$

![](_page_10_Figure_4.jpeg)

This magnetic field will lead to the spin Larmor precession

#### **START**

□ The Hamiltonian describing the S-O interaction is obtained from the non-relativistic limit of the Dirac equation

$$H_{SO} = \frac{\hbar}{(2m_0c)^2} \vec{\nabla} V \cdot (\hat{\sigma} \times \hat{p})$$
Non-relativistic Dirac Hamiltonian
$$\hat{\sigma} = (\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z)$$
Pauli matrices
For a central potential
$$H_{SO} = \lambda \vec{L} \cdot \vec{S}$$

$$\vec{L}$$
Orbital momentum

=> Gives the name of the S-O interaction

$$ec{L}$$
 Orbital momentum  $ec{S}$  Spin momentum 11

(I) Starting from the non-relativistic Dirac Hamiltonian, written for the case of a 2D free- electron gas with a confinement direction perpendicular to the propagation direction, we deduce the Rashba Hamiltonian. Then we identify the SO (Rashba) constant.

□ Consider the Datta-Das transistor geometry with *E* along *OZ*<sub>ref</sub>

![](_page_11_Figure_2.jpeg)

$$(2m_0c)^2$$

Considering the 2DEG with the confinement direction perpendicular to the propagation direction, one can calculate the vector product:

$$\hat{\sigma} \times \hat{p} = \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ \hat{\sigma}_x & \hat{\sigma}_y & \hat{\sigma}_z \\ p_x & p_y & p_z \end{vmatrix}$$

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$$\hat{\sigma} \times \hat{p} = \hat{x} \left( p_z \hat{\sigma}_y - p_y \hat{\sigma}_z \right) - \hat{y} \left( p_z \hat{\sigma}_x - p_x \hat{\sigma}_z \right) + \hat{z} \left( p_y \hat{\sigma}_x - p_x \hat{\sigma}_y \right)$$

If  $\vec{E} = -\vec{\nabla}V$  is applied along  $OZ_{ref}$  axis perpendicular to the 2DEG plane, we would have:

$$\vec{\nabla}V \cdot (\hat{\sigma} \times \hat{p}) = -\frac{\partial V}{\partial z} (\hat{p}_x \hat{\sigma}_y - \hat{p}_y \hat{\sigma}_x) \qquad \Longrightarrow \qquad H_{so} = -\frac{\hbar}{(2m_0 c)^2} \frac{\partial V}{\partial z} (\hat{p}_x \hat{\sigma}_y - \hat{p}_y \hat{\sigma}_x)$$

Rashba Hamiltonian

Within the **free-electron** approach, the total Hamiltonian of an electron with the mass  $m = \Sigma$  (K+SO)

$$\hat{H}_{SO} = \frac{\hat{p}_x^2 + \hat{p}_y^2}{2m} - \frac{\hbar}{\left(2m_0c\right)^2} \frac{\partial V}{\partial z} \left(\hat{p}_x \hat{\sigma}_y - \hat{p}_y \hat{\sigma}_x\right) \qquad \Leftrightarrow \qquad \hat{H}_{SO} = \frac{\hbar^2}{2m} \left(\hat{k}_x^2 + \hat{k}_y^2\right) - \frac{\hbar^2}{\left(2m_0c\right)^2} \frac{\partial V}{\partial z} \left(\hat{k}_x \hat{\sigma}_y - \hat{k}_y \hat{\sigma}_x\right)$$

We denote:

$$\alpha_{R} = \frac{\hbar^{2}}{\left(2m_{0}c\right)^{2}} \frac{\partial V}{\partial z}$$

#### SO interaction constant (Rashba constant)

- □ is a measure of the spin-orbit interaction.
- alpha can be controlled via the external electric field (in Datta-Das spin transistor geometry).

$$\hat{H}_{SO} = \frac{\hbar^2}{2m} \left( \hat{k}_x^2 + \hat{k}_y^2 \right) - \alpha_R \left( \hat{k}_x \hat{\sigma}_y - \hat{k}_y \hat{\sigma}_x \right) \qquad \begin{array}{c} \text{TOTAL} \\ \text{Rashba Hamiltonian} \\ \end{array}$$

#### **Discussion:**

SO interaction constant (Rashba constant)

$$\alpha_{R} = \frac{\hbar^{2}}{\left(2m_{0}c\right)^{2}} \frac{\partial V}{\partial z} \qquad \qquad -\frac{\partial V}{\partial z} = E$$

□ The larger is the *E* felt by the electron, the larger is the SO-coupling

- In case of atom, *E ~Ze* => SO larger for heavy atoms: Au (Z=79), Pt (Z=78), Pd (Z=46) than for 3D atoms: Cr (Z=24), Fe (Z=26),Co (Z=27), Ni (Z=28).
- □ SO-coupling exacerbated at the metal surfaces: the breaking of the translational symmetry in surface is equivalent to a potential gradient felt by the electron => electric field.

(II) Within the Heisenberg-Dirac formalism, we solve the stationary Schrodinger equation by diagonalising the spin-orbit Hamiltonian and find the eigenvalues and the stationary eigenfunctions.

$$\hat{H}_{SO} = \frac{\hbar^2}{2m} \left( \hat{k}_x^2 + \hat{k}_y^2 \right) - \alpha_R \left( \hat{k}_x \hat{\sigma}_y - \hat{k}_y \hat{\sigma}_x \right)$$

**TOTAL** Rashba Hamiltonian

The  $\hat{k}_x, \hat{k}_y$  operator commute with  $\hat{H}$  then the eigenfunctions of the system can be:

$$\left|\Psi\right\rangle = e^{i(k_{x}x+k_{y}y)}\left(C_{1}\left|+\right\rangle+C_{2}\left|-\right\rangle\right) = e^{i\vec{k}_{\parallel}\vec{r}}\left(C_{1}\left|+\right\rangle+C_{2}\left|-\right\rangle\right)$$

 $(|+\rangle, |-\rangle)$  Represent the UP and DN states of the z component of the spin They are orthonormal

**Obs:** The z direction in the electron referential is given by the direction of the effective magnetic field  $B_{eff}$ . This represents the magnetic field quantization axis and leads to diagonal  $\sigma_z$ .

□ Within this representation we have:

(see Blundel 2)

$$\hat{\sigma}_x = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \hat{\sigma}_y = \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \hat{\sigma}_z = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

The matrix form of the Hamiltonian:

$$\hat{H} = \hat{H}_{FP} + \hat{H}_{SO}$$

Free-particle term:

$$\hat{H}_{ij} = \left\langle i \left| \frac{\hbar^2 k_{\parallel}^2}{2m} \right| j \right\rangle$$

and take into account the orhonormized condictions

 $|i\rangle, |j\rangle = |+\rangle, |-\rangle$ 

$$\Rightarrow \hat{H}_{FP} = \begin{pmatrix} \frac{\hbar^2 k_{\parallel}^2}{2m} & 0\\ 0 & \frac{\hbar^2 k_{\parallel}^2}{2m} \end{pmatrix}$$

Spin-orbit term:

$$\hat{H}_{SO} = -\alpha_R \left[ k_x \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} - k_y \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \right] = \begin{pmatrix} 0 & \alpha_R (k_y + ik_x) \\ \alpha_R (k_y - ik_x) & 0 \end{pmatrix}$$

**Total Hamiltonian:** 

$$\hat{H} = \begin{pmatrix} \frac{\hbar^2 k_{\parallel}^2}{2m} & \alpha_R \left( k_y + i k_x \right) \\ \alpha_R \left( k_y - i k_x \right) & \frac{\hbar^2 k_{\parallel}^2}{2m} \end{pmatrix}$$

Non-diagonal =>  $|+\rangle$ ,  $|-\rangle$  are not eigenstates (stationary states) of the system

#### Eigenvalues:

S:  

$$\frac{\det\left(\hat{H}-\lambda\hat{I}\right)=0}{\left(\frac{\hbar^{2}k_{\parallel}^{2}}{2m}-\lambda\right)^{2}} \Leftrightarrow \left[\frac{\frac{\hbar^{2}k_{\parallel}^{2}}{2m}-\lambda}{\alpha_{R}\left(k_{y}+ik_{x}\right)}\right]=0$$

$$\left(\frac{\hbar^{2}k_{\parallel}^{2}}{2m}-\lambda\right)^{2} = \alpha_{R}^{2}\left(k_{y}+ik_{x}\right)\left(k_{y}-ik_{x}\right)=\alpha_{R}^{2}\left(k_{y}^{2}+k_{x}^{2}\right)=\alpha_{R}^{2}k_{\parallel}^{2}}$$

$$\lambda = \frac{\hbar^{2}k_{\parallel}^{2}}{2m}\pm\alpha_{R}\left|k_{\parallel}\right|$$

$$E_{\pm}(k_{\parallel}) = \frac{\hbar^2 k_{\parallel}^2}{2m} \pm \alpha_R \left| k_{\parallel} \right|$$

$$\left( \swarrow \left( \vec{k} \cdot S_{\perp} \right) = \frac{\pi}{2m} \right)$$

$$\begin{cases} \mathcal{L}\left(k_{\parallel}, S_{|\Psi-\rangle}\right) = \frac{\pi}{2} \\ \mathcal{L}\left(\vec{k}_{\parallel}, S_{|\Psi+\rangle}\right) = -\frac{\pi}{2} \end{cases}$$

- □ The eigenvalues of the Rashba Hamiltonian
- □ Correspond to a 2 state system (spin parallel and antiparallel to B<sub>eff</sub>)

![](_page_16_Figure_6.jpeg)

**G** SO influence on the parabolic E(k) band structure

□ How the spin-orbit constant alpha can be extracted from ARPES experiments.

**OBS:** Because  $\alpha_R$  is small (1 order of magnitude smaller than  $E_F$ ) high resolution of analizer is required in photoemission experiments to observe the split

$$\alpha_R = 1meV \rightarrow \Delta k \sim 10^{-15} m^{-1} = 10^{-5} Å^{-1}$$

![](_page_18_Figure_0.jpeg)

Electron photoemission experiments on a 2D electron (Shockley) state on Au(111) surface –*G. Nicolay, F. Reinert, S. Hufner, P. Blaha, Phys. Rev. B* 65 (2002) 033407 respectiv *F. Reinert, G. Nicolay, S. Schmidt, D. Ehm, S. Hufner, Phys. Rev. B* 63 (2001) 115415. The experimens are taken at 30K. Bottom panel: the band structure  $E(k_x)$  along the  $\overline{\Gamma M}$  direction.

Middle panel: cut on  $(k_{x_y} k_y)$  representation (top panel) at  $k_y = 0$ 

 $\Box$   $\alpha_R$  from ARPES for materials with important potential in spin-orbitronics (when materials with significant SO are used for generation of spin currents by spin-Hall effects).

![](_page_19_Figure_1.jpeg)

From A. Fert

### Eigenfunctions

The general form of the eigenfunctions within the  $\{|+\rangle,|-\rangle\} \text{ basis is:}$ 

$$\left| \Psi \right\rangle = e^{i\vec{k}_{\parallel}\vec{r}} \left[ u \left| + \right\rangle + v \left| - \right\rangle \right]$$

 $\left(\hat{H} - \lambda \hat{I}\right) \begin{pmatrix} u \\ v \end{pmatrix} = 0$ 

Where the amplitude probabilities  $\boldsymbol{u}$  and  $\boldsymbol{v}$  verify the matrix equation:

**Obs:** The states  $|\Psi_{{\scriptscriptstyle E^+}}
angle$ ,  $|\Psi_{{\scriptscriptstyle E^-}}
angle$  are stationary states of the system

□ Furthermore, we study the time evolution, solving the time dependent Schrodinger equation. Then, by calculating average values of the spin operators Sx, Sy, Sz we can demonstrate and discuss the spin precession.

To describe the time evolution of the system we use the expression of the solution of the

Schrodinger equation projected on the  $\{|\Psi_{E^+}\rangle, |\Psi_{E^-}\rangle\}$  basis:

![](_page_21_Figure_3.jpeg)

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If one define the amplitudes of probability:

$$\left\|\Psi(t)\right\rangle^{2} \rightarrow \begin{cases} \left|C_{1}(t)\right|^{2} \propto \cos^{2}\frac{\alpha_{R}k_{\parallel}}{\hbar}t\\ \left|C_{1}(t)\right|^{2} \propto \sin^{2}\frac{\alpha_{R}k_{\parallel}}{\hbar}t \end{cases}$$

![](_page_22_Figure_3.jpeg)

Flip-flop movement betwen the two unstationary states:

$$|+\rangle, |-\rangle$$

#### **Precession with Larmor frquency**

In order to demonstrate the spin precession, one has to calculate the average values of the spin operatos:  $\langle \hat{S}_x(t) \rangle, \langle \hat{S}_y(t) \rangle, \langle \hat{S}_z(t) \rangle$  within the basis:  $\{ |\Psi_{E^+} \rangle, |\Psi_{E^-} \rangle \}$ 

$$\left|\Psi(t)\right\rangle = \frac{e^{i(\vec{k}_{\parallel}\vec{r}-\omega_{0}t)}}{\sqrt{2}} \left\{ e^{\frac{i\theta}{2}} \cos\frac{\alpha_{R}k_{\parallel}t}{\hbar} \right| + \left| -ie^{-\frac{i\theta}{2}} \sin\frac{\alpha_{R}k_{\parallel}t}{\hbar} \right| - \left| \right\rangle \right\} = C_{+}(t) \left| + \right\rangle + C_{-}(t) \left| - \right\rangle$$

$$\left\{ C_{+}(t) = e^{\frac{i\theta}{2}} \frac{e^{i(\vec{k}_{\parallel}\vec{r}-\omega_{0}t)}}{\sqrt{2}} \cos\frac{\alpha_{R}k_{\parallel}t}{\hbar} \right\}$$

$$\left\{ C_{-}(t) = -ie^{-\frac{i\theta}{2}} \frac{e^{i(\vec{k}_{\parallel}\vec{r}-\omega_{0}t)}}{\sqrt{2}} \sin\frac{\alpha_{R}k_{\parallel}t}{\hbar} \right\}$$

$$\langle \hat{S}_{z} \rangle = \langle \Psi | \hat{S}_{z} | \Psi \rangle = \frac{\hbar}{2} (C_{+}^{*} C_{-}^{*}) \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} C_{+} \\ C_{-} \end{pmatrix} = \frac{\hbar}{2} [C_{+}^{*} C_{+} - C_{-}^{*} C_{-}]$$

$$\left\langle \hat{S}_{x}\right\rangle = \left\langle \Psi \right| \hat{S}_{x} \left| \Psi \right\rangle = \frac{\hbar}{2} \begin{pmatrix} C_{+}^{*} & C_{-}^{*} \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} C_{+} \\ C_{-} \end{pmatrix} = \hbar \Re e \begin{bmatrix} C_{+}^{*} C_{-} \end{bmatrix}$$

$$\left\langle \hat{S}_{y} \right\rangle = \left\langle \Psi \right| \hat{S}_{x} \left| \Psi \right\rangle = \frac{\hbar}{2} \begin{pmatrix} C_{+}^{*} & C_{-}^{*} \end{pmatrix} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} C_{+} \\ C_{-} \end{pmatrix} = \left\langle \hat{S}_{y} \right\rangle = \hbar \Im m \begin{bmatrix} C_{+}^{*} & C_{-} \end{bmatrix}$$

The period of this precession is:

$$T = \frac{2\pi}{\Omega} = \frac{\pi\hbar}{\alpha_{\rm R}k_{\rm H}}$$

Precession equations of the spin angular momentum  $\boldsymbol{S}$  with the frequency  $\Omega$  analoguous to the Larmor precession around  $B_{eff}$ 

To be dephased with  $\pi$ , the spin has to travel a distance corresponding to a half-period:  $T_L = \frac{\pi \hbar}{2\alpha_R k_{\parallel}}$ 

In the Datta@Das transistor, the distance between source and drain is adjusted to insure the rotation with  $\pi$  whe E of the gate is turned on <sup>25</sup>

![](_page_25_Figure_0.jpeg)

Vector diagram within the lab referential

Vector diagram within the electron referential