B. Halperin   Spin lecture 1

Spins and spin-orbit coupling in semiconductors, metals, and nanostructures

Behavior of non-equilibrium spin populations.

Spin relaxation and spin transport.

How does one produce and detect non-equilibrium spin populations. How can one manipulate non-equilibrium spins?

Emphasis on the role of spin-orbit coupling in semiconductor systems.

Spin-subjects discussed by previous speakers include:

Ferromagnetic-nonmagnetic metal hybrid structures. (Dan Ralph) Use of electric currents to detect or alter the orientation of magnetic domains.

Role of spin-orbit coupling in Random Matrix Theory and in electrical resistance at low temperatures: weak antilocalization and reduced conductance fluctuations in two-dimensional systems and quantum dots (Altshuler, Marcus,Birge)

Motivations for study of non-equilibrium electron spins include possibilities of practical applications.

Systems based on ferromagnets are very important for data storage and retrieval-magnetic memory devices including hard discs and magnetic random access memories GMR read heads.

Reversal of magnetic domains is currently accomplished by applying magnetic fields. If one can control orientation directly with electrical currents or electric fields, that could be useful: they are much easier to apply locally in nanoscale geometries.

Magnetic information is typically converted to charge information (variations in voltages, electrical currents) for further data processing.Perhaps it could be useful to process information with spins directly.

As discussed by Charlie Marcus:
Electron spins in semiconductor nanostructures are one possibility for qubits in a quantum computer.

How to produce a non-equilibrium spin population

Injection from a ferromagnet to a normal metal or semiconductor, through an interface; via electrical currents, or optical excitation.

Creation of electron-hole pairs by circularly polarized light above the band gap of semiconductor.

Electrical transport through a quantum dot in an applied magnetic field

Use of electrical currents to generate spin currents and polarization without magnetic fields or ferromagnets, via **spin-orbit coupling**.

How to detect a non-equilibrium (or equilibrium) spin polarization

Electrical resistance at a ferromagnet-nonmagnetic interface can depend on spin polarization in non-magnetic metal, as well as orientation relative to ferromagnet..

Spin polarization can lead to Faraday rotation of light, in transmission or reflection..

Transmission through a quantum dot or nanostructure in an applied magnetic field can depend on spin of incident electrons.

Electrical resistivity of a bulk material can depend on degree of spin polarization.

Electrical current in spin-polarized material can generate Hall voltage due to Anomalous Hall Effect, arising from spin orbit coupling.

How to manipulate (rotate) spin polarizations

With applied magnetic fields:

Electron spin resonance.

With applied electric fields via spin-orbit coupling.

With time-dependent optical beams.

Via coupling to nuclei.

Sources of spin relaxation

Spin-orbit coupling.

Coupling to nuclear spins.

Origins of Spin-Orbit Coupling

Microscopic Hamiltonian, electron in potential V:

$$H = (p^2/2m) + V(\mathbf{r}) + \lambda_0 \, \boldsymbol{\sigma} \cdot (\mathbf{p} \times \nabla V) \; ,$$

$$\lambda_0 = -\hbar /(4 \, m^2 c^2) = -3.7 \times 10^{-8} \text{ nm}^2 \; .$$

Comes from Dirac equation, first spin-dependent term in relativistic expansion. (For heavy atoms, electron velocity can approach c near nucleus, should use full Dirac equation).

In system with many electrons, replace V with self-consistent potential. Many body corrections to SO are relatively small. Other relativistic effects which couple spin and orbital motion include magnetic dipole-dipole interaction between spins and interaction between spin of one electron with orbital magnetic moments of others.

Spin orbit effects in atoms or ions

Spin orbit effects are most important when they split a degeneracy of the non-relativistic atom. For light atoms (Z < 70) use Russel-Saunders (LS) coupling. First: find non-relativistic ground state, *including electron-electron interactions*, If total orbital angular momentum L and total spin S are both non-zero, find states with different total angular momentum J ($\mathbf{J} = \mathbf{L} + \mathbf{S}$), have different energies.

Hunds rule: If outer shell is more than half full, ground state has J=L+S. Magnetic moment $\mathbf{M} \propto \mathbf{L} + 2\mathbf{S}$, -> Lande g-factor satisfies 1 <g < 2.

If outer shell is less than half full, J = |L-S|. Lande g factor can be bigger than 2.

Magnetic ion in a crystal

An ion embedded in an insulating crystal may have a degenerate ground state, with broken time reversal symmetry, and therefore may have a magnetic moment.

Orbital angular momentum is not a good quantum number, but depending on symmetry of lattice site, ground state may still have orbital degeneracy.Ion will have local magnetic moment which is a combination of spin and orbital angular momentum, g-factor may be far from 2, and may be strongly anisotropic. (We still describe the ground state degeneracy and the magnetic moment as due to a "spin". If two-fold degenerate, describe by Pauli spin matrices.) If orbital ground state is non-degenerate, magnetic moment will be mostly spin, g-factor will be close to 2, close to isotropic.

Exchange interactions in magnetic insulators.

In the absence of spin-orbit coupling, the exchange interaction between spins must have Heisenberg symmetry:

$$H_{spin} = \Sigma_{i,j} \; J_{ij} \; \mathbf{S}_i \cdot \mathbf{S}_j \; .$$

Invariant under simultaneous rotations of the spins.

With spin orbit coupling, exchange may be anisotropic, depending on orientation relative to the crystal axes, and the line joining the spins. In simplest case may have Ising-like or XY-like symmetry

$$H_{spin} = \Sigma_{i,j} \; [J_{ij}{}^z \; S_i{}^z \; S_j{}^z \; + J_{ij}{}^x \; (S_i{}^x \; S_j{}^x + S_i{}^y \; S_j{}^y) \;]$$

Spin-orbit effects on band-structure:

Non-interacting electrons in a self-consistent periodic potential V($\mathbf{r}$)

$$H = (p^2/2m) + V(\mathbf{r}) + \lambda_0\,\boldsymbol{\sigma}\cdot(\mathbf{p}\times\boldsymbol{\nabla}V)$$

Bloch's theorem: $\psi_{nk\alpha}(\mathbf{r},\sigma) = e^{i\mathbf{k}\cdot\mathbf{r}}\,u_{nk\alpha}(\mathbf{r},\sigma)$, where u is periodic. $\alpha = \pm 1$ is a (pseudo)spin index..

Without spin-orbit coupling: $u_{nk\alpha}(\mathbf{r},\sigma) = u_{nk}(\mathbf{r})\,\delta_{\alpha\sigma}$, and energy $\varepsilon_{nk\alpha} = \varepsilon_{nk}$

With spin orbit coupling ....

Symmetry considerations

Kramers Degeneracy. Time reversal symmetry requires

$$\varepsilon_{nk\alpha} = \varepsilon_{n,-k,-\alpha} \ , \qquad u_{nk\alpha}(\mathbf{r},\sigma) = \sigma \, u^*_{n,-k,-\alpha}(\mathbf{r},-\sigma) \ .$$

If crystal has inversion symmetry, $\varepsilon_{nk\alpha} = \varepsilon_{n,-k\,\alpha}$,

$$\text{hence } \varepsilon_{nk\alpha} = \varepsilon_{nk,-\alpha}$$

(2-fold degeneracy at each k-point separately.)

If no center of inversion: energy levels at a given **k** are split by an amount b(**k**), except at special symmetry points, where b -> 0.

Splitting is generally small, but can have interesting effects

General size of spin-orbit effects on band structure

Spin-orbit effects generally give small corrections to the non-relativistic band structure, except near **k**-points where bands are degenerate in the non-relativistic structure..

Important examples of this are:

At the hexagonal face of the Brillouin zone for an hcp metal.

Near the valence-band maximum, at the zone center (Γ-point) of a group IV or zincblende III-V semiconductor: (Si, Ge, GaAs, etc).
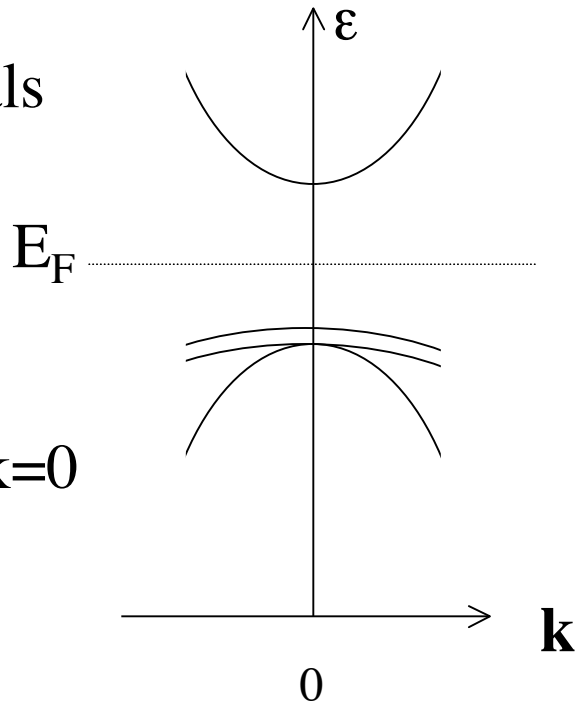
GaAs near k=0

GaAs near k=0

Antibonding s orbitals

Bonding p orbitals.
3-fold degenerate at k=0

Also applies to Si and Ge, but in those cases the k=o minimum is not the lowest point of the conduction band..
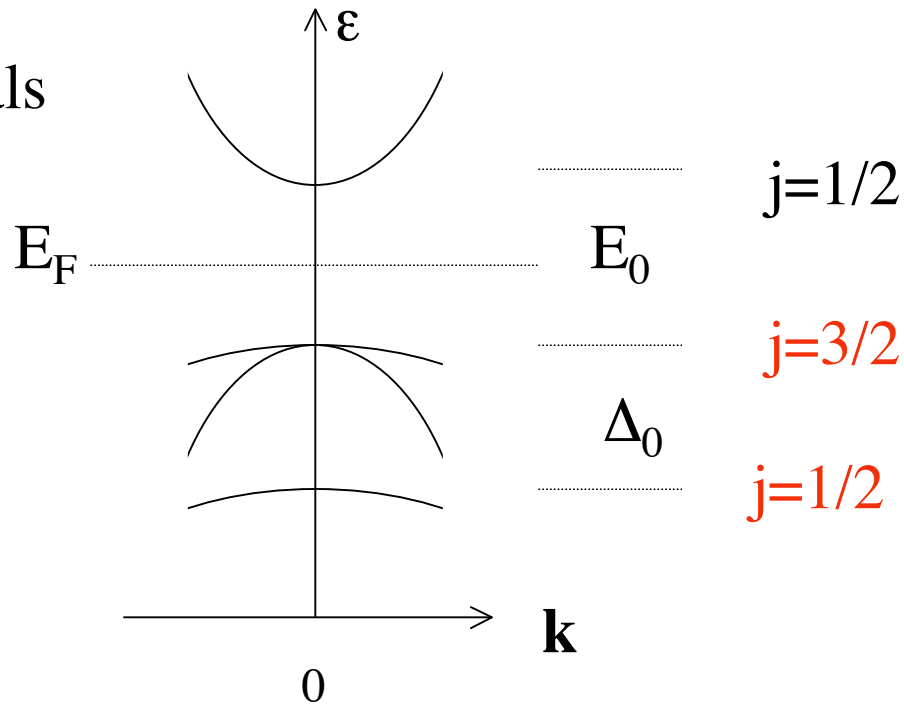
GaAs near k=0

With spin orbit

Conduction band

Antibonding s orbitals

Bonding p orbitals

Valence band

Neglects broken inversion symmetry in GaAs.
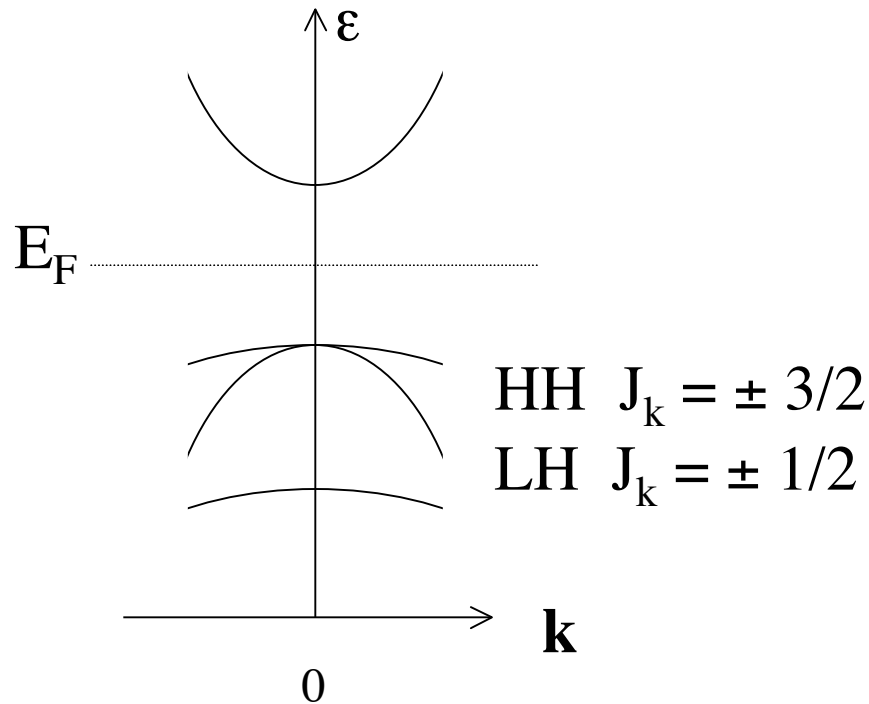
Also applies to Si and Ge

GaAs near k=0

Effective Hamiltonian

Conduction band

$$H = E_o + k^2/2m$$

ε

E_F

Valence band

$$H = -(k^2/2m_v) + C(\mathbf{k} \cdot \mathbf{J})^2$$

HH $J_k = \pm 3/2$

LH $J_k = \pm 1/2$

$\mathbf{k}$

0

Heavy and light hole masses are given by $m_H^{-1} = (m_v^{-1} - 2C)$ and $m_L^{-1} = (m_v^{-1} + 2C)$.

Neglects cubic anisotropy and broken inversion symmetry.

2D hole gas in GaAs

Assume square confining well. Neglect broken inversion symmetry and cubic anisotropy.

$H = -(k^2/2m_v) + C(\mathbf{k} \cdot \mathbf{J})^2$ with $k_z^2 = (\pi/d)^2$, $\langle k_z \rangle = 0$.

4x4 matrix has 2 pairs of degenerate eigenvalues

Top of valence band has $J_z = \pm 3/2$ at k=0. (Heavy holes in z-direction). Light hole band ($J_z = \pm 1/2$) has higher energy by amount $2C (\pi/d)^2$. Away from k=0, bands are mixed. Perturbation $C(k_x J_x + k_y J_y)^2$ enters only in second order perturbation theory. So close to k=0, effective Hamiltonian is

$H_{eff} = -E_c -(k^2/2m_v)$, where the confinement energy is

$E_c = 9(\pi/d)^2/8m_H$.

Effects of a magnetic field

Replace **k** by **k** - e **A**(**r**)/c .

Add Zeeman term H_Z which splits spin degeneracy.

For electrons in conduction band, $H_Z = -(g\mu_B/2)$ **B·σ** , where the Pauli spin matrices **σ** $= (\sigma_x, \sigma_y, \sigma_z)$ act on the (pseudo)spin index $\alpha. = \pm 1$. (In GaAs, g=-0.41)

For holes in bulk GaAs, $H_Z \propto$ **B·J** (4x4) matrix.

For 2D holes gas in GaAs, we wish to consider only the two states in the heavy hole band which are separated from the light hole band by the difference in confinement energies. Use pseudospin index $\propto = \pm 1$ to label states which have $J_z = \pm 1$ at k=0. Defining Pauli spin matrices **σ** to act on index α, we find very anisotropic g-factor: $H_Z \propto B_z \sigma_z$. Coupling to in-plane field is $\propto k^2$.

Effects of Broken Inversion Symmetry

For band which is 2-fold degenerate in absence of broken inversion symmetry, we write $H_{SO} = - \mathbf{b}(\mathbf{k}) \cdot \boldsymbol{\sigma} / 2$.

For conduction electrons in bulk GaAs, $\mathbf{b}$ has the form (Dresselhaus coupling) :

$$b_x = \gamma \, k_x(k_y^2 - k_z^2) + \text{cyclic permutations.}$$

For a 2DEG in a symmetric confining well, set $k_z^2 = (\pi/d)^2$, $<k_z> = 0$, obtain

$b_x = - \beta k_x + \gamma \, k_x k_y^2 , \quad b_y = \beta k_y - \gamma \, k_y k_x^2 ,$ with

$\beta = \gamma \, (\pi/d)^2$.

For a 2DEG in an asymmetric confining well, get additional (Rashba) term: $\mathbf{b}(\mathbf{k}) = \alpha \; \mathbf{z} \times \mathbf{k}$.

Effects of Broken Inversion Symmetry (continued)

For holes in bulk GaAs, lack of inversion symmetry leads to a splitting of the four hole bands which is linear in k near k=0, but is very small.. Similarly, intrinsic inversion asymmetry of GaAs has small effect in 2D hole gas.

For 2D hole gas in an asymmetric confining well, we again find a Rashba term, which we may write as

$H_{SO} = - \mathbf{b(k)} \cdot \mathbf{\sigma} /2$, with $b_z = 0$, but now

$$(b_x + ib_y) = \alpha (k_x + ik_y)^3 .$$

Scattering by impurities

Even if the host material has inversion symmetry, defects or impurities add perturbations which can mix states of different pseudospin.For an impurity potential V which varies slowly on the scale of the lattice constant, within the effective mass approximation, we may write:

$$H = (k^2/2m^*) + V(\mathbf{r}) + \lambda \, \boldsymbol{\sigma} \cdot (\mathbf{k} \times \nabla V) .$$

This is the same form as in vacuum but λ depends on the host material. For the conduction band of GaAs. $\lambda = 0.053 \text{ nm}^2$, which is 10^6 times larger than the vacuum value

$\lambda_0 = -3.7 \times 10^{-8} \text{ nm}^2$

Relaxation of spin
Elliott-Yafet mechanism

For a material with inversion symmetry, in the absence of scattering, the psuedospin σ is a constant of the motion. However, scattering by impurities or phonons can flip the pseudospin. For $H_{SO} = \lambda\, \sigma \cdot (\mathbf{k} \times \nabla V)$, the scattering amplitude in the first Born approximation has a contribution proportional to $i\lambda\, \sigma \cdot (\mathbf{k} \times \mathbf{k}')V(\mathbf{k} - \mathbf{k}')$, This leads to a spin relaxation rate

$$\tau_{sf}^{-1} \propto (\lambda\, k_F)^2\, \tau_{tr}^{-1},$$

where τ_{tr}^{-1} is the transport scattering rate.

$(\lambda\, k_F)^2$ is of order 10^{-3} for electrons in GaAs.

Relaxation of Spin
Dyakonov-Perel Mechanism

In a system with broken inversion symmetry, the spin-orbit field **b(k)** causes the components of pseudospin perpendicular to **b** to precess at a frequency b. The component parallel to b is conserved until the electron is scattered through an angle large enough to change the direction of **b**. If In the "clean limit", where $b\tau_{tr} \gg 1$, spin memory will persist for times of order τ_{tr}

In the "dirty limit", where $b\tau_{tr} \ll 1$, the field direction seen by an electron changes rapidly, and the spin direction diffuses over the unit sphere, with a relaxation rate

$$\tau_{sf}^{-1} \propto b^2 \tau_{tr} .$$

How do you understand structure and parameters?

k · p perturbation theory

4 x 4 Hamiltonian for valence band (Luttinger model)

8 x 8 Hamiltonian (Kane model)

14 x 14 Hamiltonian (includes antibonding p orbitals in conduction band)

Reference: R. Winkler, "Spin-Orbit Coupling effects in Two-Dimensional Electron and Hole Systems", (Springer, 2003)