Module 2: Magnetoelectronics
Lecture 06: Electronic structure of normal metals

Magnetoelectronics:
We are familiar with electronic devices which exploit the two charge carriers - electrons and holes in semiconductor to build devices. A new concept, which is rapidly merging into a reality, is the use of spin – up-spin and down-spin in a similar way to build spintronic devices. Magnetoelectronics is a sub-set of this new paradigm which concerns use of the spins in magnetic materials for such applications. In this chapter, the underlying principles behind this branch of magnetoelectronics would be introduced using the electronic structure of metals. The valance electrons in metals are delocalized and are called conduction electrons since they are involving the conduction process. These electrons can wander freely through the sample and are also known as itinerant electrons. In some cases the magnetic moments in metals are associated with the conduction electrons. In other cases, the magnetic moments remain localized. In both these cases paramagnetic and diamagnetic behaviours can occur. Ferromagnetism is possible under certain conditions. The itinerant theory of magnetism based on free electron theory is applicable to the magnetism of 3d series of elements such as iron, cobalt and nickel. The free electron model is a crude approximation to most real situations, but it is simple to consider and will allow the discussion to proceed a long way. The itinerant conduction band theory of paramagnetism developed by Pauli helps in understanding the influence of magnetic field on magnetization of a paramagnetic metal. This would then lead to a discussion on the band picture of a ferromagnetic metal. With the background the spin-up and spin-down bands in a ferromagnetic metal, it becomes easy to understand a new class of spintronic materials called half-metals. A discussion on spin polarized materials and spin-dependent transport would conclude our introduction to these novel materials.

This chapter will address the following points:
1. How are the conduction electrons arranged in a normal metal in the absence of and presence of an applied magnetic field?
2. How can these ideas be generalized to understand a ferromagnetic metal which has a net magnetization?
3. What are half-metals? Why are they called spin polarized materials?
4. How to understand spin-dependent transport in a quantitative manner?
Electronic structure of normal metals

The Drude model was the first attempt made to explain the electrical properties of metals using the idea of an electron gas that is free to move between positively charged ion cores [1, 2, 3]. This over simplistic model considered only collision between the electrons and the ion cores and ignored inter-electron collisions and interactions. This attempt to apply classical kinetic theory to electrons in metals failed to correctly predict the properties of metals with its main success being the reasonably correct prediction of the Weidemann-Franz ratio of metals at room temperature. Failure of the electron gas approach was diagnosed by Sommerfeld’s model in which the electrons were treated as quantum mechanical particles. Sommerfeld replaced the classical Maxwell-Boltzmann distribution with Fermi-Dirac distribution and successfully predicted the experimentally observed temperature, dependence and magnitude of electronic specific heat, (thermal and electrical) conductivities and Weidemann-Franz ratio of metals. This model could also explain the temperature dependence of the magnetic susceptibility of metals. However, this model could not explain why certain materials are insulators or semiconductors and other experimentally observed features such as the correct value of the Hall coefficient, magneto-resistance and Seebeck coefficient. Let us use the ideas of Sommerfeld’s model to arrive at parameters relevant to understanding the electronic structure of metals.

According to quantum mechanics, we can have only certain number of states \( N \) per unit volume of phase space in three dimensions, where

\[
N = \left(\frac{1}{2\pi}\right)^3 V_{k3} V_{r3} \tag{6.1}
\]

Here, \( V_{k3} \) is the \( k \)-space volume and \( V_{r3} \) is the 3-dimensional space volume. Now assuming that electrons are free to move within the solid in a mean potential \( -V_0 \), the energy of the electrons is

\[
E(k) = -V_0 + \frac{p^2}{2m_e} = -V_0 + \frac{\hbar^2 k^2}{2m_e} \tag{6.2}
\]

where \( \hbar = h/2\pi \) is the reduced Planck’s constant and \( m_e \) is the mass of electron. If we choose a convenient origin of energy as \( E = 0 \), corresponding to the average potential within the metal, then,

\[
E(k) = \frac{\hbar^2 k^2}{2m_e} \tag{6.3}
\]
Let us now gradually put electrons into the metal. At $T = 0$, the first two electrons will occupy the lowest energy (or lowest $|k|$) state and the subsequent electrons will be forced to occupy higher and higher energy states as per Pauli’s exclusion principle. Eventually, when all the electrons are accommodated, a sphere of $k$-space would have been filled up with

$$N = 2 \left( \frac{1}{2\pi} \right)^3 \left( \frac{4\pi}{3} \right) k_F^3 V_r$$

(6.4)

Where $k_F$, the Fermi wavevector is the $k$-space radius of the sphere of filled states. The factor 2 in the above equation denotes the spin degeneracy of the electron. Substituting $n = N/V_r$ in the above equation gives,

$$k_F = (3\pi^2 n)^{1/3}$$

(6.5)

The corresponding energy is then

$$E_F = \frac{\hbar^2 (3\pi^2 n)^{2/3}}{2m_e}$$

(6.6)

This highest filled electron energy is known as Fermi energy.

Substituting typical values of parameters corresponding to electrons in metals in the above equation yields $E_F$ values in the range of ~1.5 to 15 eV or $E_F/k_B = ~20 \times 10^3$ K to $100 \times 10^3$ K, which is very much higher than room temperature. The velocity of electrons at the Fermi surface is $v_F = \hbar k_F/m_e \sim 0.01c$. Although the Fermi surface at $T = 0$ is the ground state of the electron system, the electrons present are enormously energetic.

A function which describes the number of electron states in a particular energy range is very useful. To arrive at this expression let us consider eqn.(6.4) with a general value for $k$ rather than $k_F$. Such an expression gives $n(k)$, the number of states per unit volume of $r$-space with wavevector less than $|k|$. For free electrons, with energy $E = \hbar^2 k^2/2m_e$, one can then define a density of states $g(E)$, where $g(E)dE$ is the number of electrons per unit volume of $r$-space with energies between $E$ and $E + dE$:

$$g(E) = \frac{dn}{dE} = \frac{dn}{dk} \frac{dk}{dE} = \left( \frac{1}{2\pi^2} \right) \left( \frac{2m_e}{\hbar^2} \right)^{3/2} E^{1/2}$$

(6.7)

Since only the electrons within $\sim k_B T$ are capable of taking part in thermal processes, only the density of electron states (DOS) at the Fermi energy $E_F$ will be of importance. Taking natural logarithm of the expression for $E_F$ [eqn.(6.6)] gives

$$\ln(E_F) = \frac{2}{3} \ln(n) + constant$$

(6.8)
Differentiating the above expression yields,

\[
\frac{dE_F}{E_F} = \frac{2\,dn}{3\,n}
\]  \hspace{1cm} (6.9)

Rearranging and using eqn.(6.7) gives

\[
\frac{dn}{dE_F} = g(E_F) = \frac{3}{2}\frac{n}{E_F}
\]  \hspace{1cm} (6.10)

which is the electronic DOS at \(E_F\).

References:
Module 2: Magnetoelectronics
Lecture 07: Ferromagnetic metals and Half metals

All metals exhibit a weak paramagnetism which is temperature independent. This type of magnetism, known as Pauli paramagnetism, can be explained by the above model (see Fig.7.1). When a magnetic field is applied to a metal, the orientation of the magnetic moments of the electrons is constrained to be either parallel or antiparallel to the field direction.

Figure 7.1: Spin-up and spin-down state separation in a metal as per Pauli paramagnetism in the (a) absence of applied field \((H = 0)\) and (b) in the presence of field \((H > 0)\).

Since the energy of the electron in either of the orientations is different, this leads to the splitting of the parallel and antiparallel energy states. Electrons with magnetic moment \(m\) parallel to the field direction have energies reduced by \(\Delta E = -\mu_B m H = -\mu_B H\) (where \(-\mu_B\) is the Bohr magnetron), while those in antiparallel orientation will have energies increased by \(\Delta E = \mu_B m H = \mu_B H\). Some of these antiparallel electrons can reduce the energy of the system by occupying parallel states of lower energy. The numbers of electrons which can change orientation and still reduce the total energy are those which were within \(\mu_B m H\) of \(E_F\) in the absence of the field. The Pauli paramagnetic susceptibility \(\chi_p = M H\), where \(M\) is the magnetization of magnetic moment per unit volume, is

\[
\chi_p = 2m \frac{dn(E_F) \Delta E}{dE} H
\]  

\(7.1\)
Since $\Delta E/H = \mu_0 m$,

$$\chi_p = 2\mu_0 m^2 g(E_F)$$  \hspace{1cm} (7.2)$$

$\chi_p \approx 10^{-10}$ and is dependent entirely on the small fraction of electrons residing close to $E_F$.

**Ferromagnetic metals and Half-metals**

As discussed in the earlier sections, magnetism in materials mainly arises due to the spin and orbital motion of electrons. It has also become obvious that interaction of electrons with the ions cannot be ignored for understanding the electronic properties of solids. This led to the modeling of electron motion in a periodic square potential created by the regular arrangement of positive ions in a crystal. When atoms are brought together to form a solid, their atomic orbitals overlap leading to closely spaced electron energy levels. The separation between the electron energy levels decrease, leading to groups of very closely spaced (almost continuous energy states) or allowed energy bands separated by unallowed energy gaps or forbidden energy gap. The closely spaced electron states within a band can be filled with electrons according to Pauli’s principle of occupancy of electrons in each closely space energy level. Depending upon the number of electrons available in the solid, one would end up filling several of these bands, fully in some cases and partially in others. Electrons in highest filled/partially filled bands can only contribute to conduction. The highest filled band is called the valance band and the highest partially filled band is called the conduction band. As the name suggests electrons in conduction band contribute to the conduction process. Metals are solids with partially filled conduction band and hence are good conductions. Band structure of metals and semiconductors are schematically depicted in Fig. 7.1. This is the essence of the band theory of solids. The localized or atomic theory and the itinerant or band theory are the two extreme case models used for understanding the magnetization of solids. The itinerant model, in which the magnetic moments are considered to be due to conduction band electrons is considered to be appropriate for $3d$ transition elements iron, cobalt and nickel, which are ferromagnetic elements [1].

![Figure 7.1: Typical band structure of (a) metals showing partially filled conduction band (CB), and (b) semiconductors, showing a small energy gap ($E_g = 1$ to $2$ eV) separating the completely filled (valence band, VB) and empty (conduction band, CB)](image)
The band theory of ferromagnetism is an extension of Pauli’s itinerant theory of paramagnetism to ferromagnetism with the inclusion of an exchange interaction (internal effective magnetic field) to align the electrons in a cooperative manner in the absence of an external applied field. This causes a relative displacement of the spin-up and spin-down half-bands called the exchange splitting. This is qualitatively similar to the scenario encountered in paramagnetism under applied field. However, in the case of ferromagnetism, the shift in energy is much larger and it occurs in the absence of the applied field! The net spontaneous magnetization is determined by the difference in the occupancy between the spin-up and spin-down states.

**References:**

Module 2: Magnetoelectronics
Lecture 08: Ferromagnetic metals and Half metals

In 3d elements, the outer electron bands are 3d (up to 10 electrons) and 4s (up to 2 electrons). In Fe, Co and Ni, the 4s band is completely filled and hence the unfilled 3d band determines their magnetic properties. Ni atoms have 8 electrons each in partially filled 3d band. Now, consider Ni crystal with $10^{29}$ atoms/m$^3$. It will have $8 \times 10^{29}$ electrons in 3d band and they will be occupying the lowest available energy states. With no interaction between the electrons, these electrons will be equally distributed in the two (spin-up and spin-down) sub-bands ($3d^{\uparrow}$ and $3d^{\downarrow}$) with no net magnetic moment, just as in the case of Pauli’s paramagnetism. So in order to get a net imbalance of spin required for ferromagnetism, one has to invoke an exchange interaction energy which can displace the energies of the spin-up and spin-down half-bands even in the absence of an external field. This exchange interaction is quantum mechanical in origin. Using the ideas of Weiss, this can also be modeled in terms of a classical mean field. This effective field is extremely large, typically about $10^9$ Am$^{-1}$ (or $10^7$ Oe). The exchange interaction has the effect of reducing the energy of parallel alignment of spins even in the absence of an external applied field. So, the occupancy of the spin-up state is energetically favoured over the spin-down state in zero field leading to a net magnetic moment. As per Heisenberg’s model, the exchange interaction energy [1],

$$ E_{ex} = -J_{ex} S_1 \cdot S_2 $$

where $J_{ex}$ Heisenberg’s exchange integral (or simply the exchange operator) and $S_1$ and $S_2$ are the electron spins. When $J_{ex} > 0$, parallel alignment is favoured leading to minimization of $E_{ex}$ and thus leading to ferromagnetism. But this can occur only when

$$ |E_{ex}| \geq \Delta E $$

Figure 8.1: Occupancy of conduction band of itinerant electron ferromagnet with (a) no exchange interaction and so net $m = 0$, and (b) with exchange interaction, leading to imbalance and net $m = 0.2 \mu_B/atom$. 

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where $\Delta E$ is the energy difference between the lowest available spin-up state and the highest occupied spin-down state. This condition ensures that any change in orientation of electronic magnetic moment causes a reduction in the total energy of the system. Fig. 8.1 shows the occupancy of the conduction band energy levels in an itinerant electron ferromagnet without and with exchange interaction.

![Diagram showing energy levels and DOS](image)

**Figure 8.2:** Electronic structure near $E_F$ of (a) a paramagnet, (b) a ferromagnet and (c) a ferromagnetic half-metal. $P$ is the electron spin polarization as defined by eqn. (8.3).

Fig. 8.2(a, b) show the electronic band structure of a paramagnet and ferromagnet near the Fermi level $E_F$. $D^\uparrow$ and $D^\downarrow$ represent the DOS of the spin-up and spin-down half-bands. Spintronics or spin electronics is an emerging area of science and technology which aims at using and manipulating the spin-up and spin-down electrons in materials for developing spin-based electronic devices. The electron-spin polarization which is defined as

$$P = \frac{D^\uparrow (E_f) - D^\downarrow (E_f)}{D^\uparrow (E_f) + D^\downarrow (E_f)}$$

which is basically a dimensionless quantity that is dependent on the DOS of the spin-up and spin-down bands at $E_F$. It can be easily understood from Fig. 8.2(a) that $P = 0$ for a paramagnet, essentially due to the equal occupancy of its spin-up and spin-down states. The net magnetization in a ferromagnet ensures that $P < 1$ as depicted in Fig. 8.2(b). This analysis shows that these two materials cannot provide spin polarized currents suitable for constructing a spintronic device. A close look at the unusual electronic structure shown in Fig. 8.2(c) will reveal a different story. The spin-up half-band in this novel band structure near $E_F$ looks similar to the spin-up half-band of a paramagnetic or ferromagnetic metal. However, the spin-down half-band resembles the spin-down band of a typical semiconductor! So, this structure depicts a material which has both metallic and semiconducting characters, the former in the spin-up half-band and the latter in the spin-
down half-band. It can also be seen that the $D_{\uparrow}(E_F)$ contribution is zero for such a band structure, resulting in $P = 1$, i.e., there are only electrons with spin-up state at $E_F$. This shows that the electrons involved in transport in materials with such band structure are 100% spin-up polarized. Materials with such peculiar band structure are called ‘half-metals’ or half-metallic materials [2,3]. Half-metallicity was first demonstrated in half-Heusler alloy NiMnSb by de Groot et al in 1983 [4]. Full-Heusler alloy Co$_2$MnSi and several other Heusler and oxide materials have been found to exhibit half-metallic nature with varying $P$ values.

References:

Quiz:
[1] What improvement did Sommerfeld do to the Drude model?
[2] What is Fermi energy?
[3] Use the value of $n$ corresponding to Na and Cu and estimate the Fermi energy levels in Na and Cu crystals.
[4] Where are the Fermi energy levels located in a metal and a semiconductor?
[5] What change does the interaction between electrons bring about in the electron occupancy of the conduction and of an ferromagnet?
[6] What type of ordering exists in a magnetic material when $J_{ex}$ is positive or negative?
[7] What is a half-metal?
[8] What is the significance of the electronic spin polarization $P$?
Module 2: Magnetoelectronics
Lecture 09: Spin dependent scattering

Objectives:
Novel magnetotransport phenomena such as giant magnetoresistance (GMR) (in magnetic multilayers) and tunnel magnetoresistance (TMR) (in ferromagnetic tunnel junctions) appear when the size scale of the magnetic materials becomes nanolevel. Therefore, it is required to understand the spin-dependent scattering process in magnetic multilayer structure and here we shall cover the spin dependent scattering process in multilayer structure films.

Spin dependent scattering of electrons:
At first, we shall focus on different types of scatterings that the electrons may experience in magnetic multilayers. In the Boltzmann equation approach, we are mainly concerned with elastic (energy conserving) scattering, i.e., in each scattering the direction of propagation of electrons changes. Therefore, it is necessary to distinguish between spin dependent and spin flip scatterings. These two types of scattering are illustrated in Fig. 9.1. In the case of spin dependent scattering the orientation of the electron spin is conserved in each scattering event but the probabilities of scattering for electrons with $\uparrow$ and $\downarrow$ spin projections are different. On the other hand, when an electron undergoes a spin-flip scattering, its spin orientation changes from $\uparrow$ ($s_Z = h/2$) to $\downarrow$ ($s_Z = -h/2$) or vice versa and, at the same time, the spin of the scattering centre changes by $\Delta = h$ so that the total spin is conserved.

There are several sources of spin flip scattering. During the fabrication process, some of the magnetic atoms may enter the non-magnetic spacer layer to form magnetic impurities. When an electron is scattered off a magnetic impurity the spins of the electron and that of the impurity can interchange provided the impurity spin is free to rotate. This occurs when the impurity spin is not strongly coupled to the spins of the ferromagnetic layers, i.e., the impurity is not near the ferromagnet / spacer interface. Electrons can also be scattered from spin waves in the ferromagnet layers. Spin waves are quasiparticles with spin one and, therefore, creation (annihilation) of a spin wave in a collision with an electron leads to a flip of the electron spin. Since it involves the spin-wave energy, this is an inelastic process which is only important at elevated temperatures. Finally, when impurities with a strong spin-orbit interaction, such as gold, are present in the multilayer, the spin of an electron incident on such an impurity may be reversed due to the spin-orbit interaction. Since all these processes mix $\uparrow$ and $\downarrow$ spin channels, they are detrimental to the large magnetoresistance.
In the case of spin dependent scattering, the key feature is that electrons with different spin orientations (↑, ↓) are scattered at different rates when they enter the ferromagnetic layers. Given that electrons obey the Pauli’s exclusion principle, an electron can be scattered from an impurity only to quantum states that are not occupied by other electrons. At zero (low) temperatures, all the states with energies \( E \) below the Fermi energy \( E_F \) are occupied and those with \( E > E_F \) are empty. Since scattering from impurities is elastic, electrons at the Fermi level can be scattered only to states in the immediate vicinity of the Fermi level. For example, the Fermi level in copper (and other noble metals) intersects only the conduction band whose density of states \( D(E_F) \) is low. It follows that the scattering probability in copper is also low. On the other hand, the \( d \) band in transition metals is only partially occupied and, therefore, the Fermi level in these metals intersects not only the conduction but also the \( d \) bands. Moreover, since the atomic wave functions of \( d \) levels are more localized than those of the outer \( s \) levels, they overlap much less, which means that the \( d \) band is narrow and the corresponding density of states is high. This opens up a new very effective channel for scattering of conduction electrons into the \( d \) band.

Figure 9.1: Schematic drawing of different types of scattering (spin dependent (left) and spin flip scatterings (right)) in magnetic multilayers.
Also, in the case of magnetic transition metals, we need to consider an additional crucial factor, namely that $d$ bands for $\uparrow$ and $\downarrow$ spin electrons are split by the exchange interaction. This amounts to an almost rigid relative shift of the $\uparrow$ and $\downarrow$ spin $d$ bands as a consequence of the fact that the potentials seen by $\uparrow$ and $\downarrow$ electrons in a ferromagnetic metal are different because of the exchange interaction. This provides another mechanism of spin dependent scattering which is specific to multilayers. In an infinite ferromagnet this effect does not lead to any spin asymmetry of the resistance since as long as the potentials seen by $\uparrow$ and $\downarrow$ electrons are periodic they do not result in any dissipation of the electron momentum. However, electrons in a multilayer entering the ferromagnet from the non-magnetic spacer see a spin dependent potential barrier which reflects differently electrons with $\uparrow$ and $\downarrow$ spin orientations. Therefore, one must seek as good a match as possible between the bands of the magnetic layers and those of the spacer layer in one spin channel and as large as possible mismatch in the other spin channel.

\[ \begin{array}{c c c c c}
\uparrow & \text{FM} & \uparrow & \text{NM} & \uparrow \\
\downarrow & \text{NM} & \uparrow & \text{FM} & \uparrow \\
\text{NM} & \uparrow & \text{FM} & \uparrow & \text{NM} \\
\text{FM} & \uparrow & \text{NM} & \uparrow & \text{FM} \\
\end{array} \]

(a) (b)

Figure 9.2: (a) FM and (b) AFM configurations of magnetic multilayers film.
Giant Magnetoresistance (GMR):

The subject of spin electronics began twenty years ago with the discovery that the electric current in a magnetic multilayer consisting of a sequence of thin FM (FM) layers separated by equally thin non-magnetic metallic layers, as shown in Figure 9.2, is strongly influenced by the relative orientation of the magnetizations of the magnetic layers. The resistance of the magnetic multilayer is low when the magnetizations of all the magnetic layers are parallel (Fig. 9.2a) but it becomes much higher when the magnetizations of the neighbouring magnetic layers are ordered antiparallel (Fig. 9.2b). This suggests that the internal magnetic moment of electrons associated with their spin plays an important role in transport of electric charge.

The optimistic magnetoresistance (MR) ratio, most commonly used is defined by

\[
\frac{\Delta R}{R} = \frac{R_{\uparrow\downarrow} - R_{\uparrow\uparrow}}{R_{\uparrow\uparrow}}
\]  

(9.1)

where \( R_{\uparrow\downarrow} \) and \( R_{\uparrow\uparrow} \) are the resistance of the multilayer film in antiferromagnetic (AFM) and FM configuration. The most commonly used combinations of magnetic and non-magnetic layers are cobalt–copper and iron–chromium but multilayers based on permalloy as the magnetic component are also frequently used. More details of the GMR are discussed in lecture 25.
Figure 9.3: Schematic arrangement of TMR junctions and the sketch of the density of states at the two sides of a magnetic junction.

**Tunnelling Magnetoresistance (TMR):**
Similar to GMR, the effect of magnetic field on the current through magnetic junctions is a subject of great interest. In particular, spin dependent tunnelling poses many interesting scientific questions, and the number of applications for magnetic junctions continues to grow. In general, the transport between two bulk metallic electrodes can be classified into two types: (a) Tunnel junction, (b) Contact junction. When the separation between the electrodes exceeds a few angstroms, electrons move between the electrodes by tunnelling. On the other hand, the two electrodes can be in contact in some points. Then, the conductance of each contact is given by $e^2/h$ times the number of electron channels through the contact.

**Magnetic Properties of the electrodes:** Since the applied magnetic field modifies the polarization of the electrodes, the density of states changes considerably (see Fig.9.3). Also, the barrier can be described in terms of an energy dependent transmission coefficient. To calculate the magnetoresistance (MR) of the junction, we just need to compare the conductance with a random orientation of the magnetization of the electrodes and that when both magnetizations are aligned. Further, we assume that

\[
\begin{align*}
D_i(E_F) &\propto N_i \\
D_\uparrow(E_F) &\propto N_\uparrow
\end{align*}
\]

where $N_\downarrow$ and $N_\uparrow$ are the number of electrons with down and up spin. Subsequently, we have

\[
\frac{\Delta G}{G_0} = \frac{G - G_0}{G_0} = \frac{(N_{1\downarrow} - N_{1L})(N_{1\uparrow} - N_{1R})}{N_L N_R}
\]

The eqn.(9.3) clearly indicates that the MR is directly proportional to the polarization of the electrodes. This simple analysis roughly explains the pioneering experiments in spin tunnelling.
**Quiz:**

(1) What are the sources available for spin-flip scattering?

(2) What is the properties one need for the ferromagnetic electrodes to get high TMR?

(3) What are the different types of GMR configurations used for devices?
Module 2: Magnetoelectronics  
Lecture 10: Spin polarization

Introduction:
The spin of the electrons will play a dominant role in the next generation electronic devices. The efficiency of such spintronic devices increases dramatically with increasing spin polarization. Therefore, the materials with a high spin polarization are of huge interest. The highest possible spin polarization is proposed for half-metals. In these materials the current is carried by the electrons that have the same spin, as demonstrated in Fig. 10.1. This is because, the half-metals exhibit a semiconducting like energy gap for the spin down electrons at the Fermi energy, which forbids the electrons having spins with down configuration. This corresponds to a spin polarization at the Fermi energy of $P = 1$. Another type of materials for which half-metallicity is proposed is the Heusler alloy with a structure of $\text{Ni}_2\text{MnIn}$. Therefore for the use of $\text{Ni}_2\text{MnIn}$ in a spin-controlled device preparation and investigation of thin films of $\text{Ni}_2\text{MnIn}$ are essential.

![Figure 10.1: Schematic representation of the density of states close to the Fermi energy for a half-metal (on the right) with respect to the normal metals and semiconductors (on the left).](image)

The determination of the spin polarization of materials is not trivial. A few methods are capable of measuring this material property, i.e., photoemission, tunnelling spectroscopy and point contact Andreev reflection (PCAR) spectroscopy.
Spin Polarization:
The spin polarization $P$ describes the different number of spin-up and spin-down electrons. The correct definition of $P$ depends on the fraction of electrons and their spins that take part in the physical process that is being investigated.

1. In a spectral generalized magneto-optical ellipsometry, all electrons are involved and the spin polarization corresponds to the total magnetization. Taking a look at the transport properties of a material, only electrons within $k_B T$ around the Fermi energy ($E_F$) and their spins are important. Therefore, the spin polarization is defined at $E_F$ as

$$P_N = \frac{N_\downarrow(E_F) - N_\uparrow(E_F)}{N_\downarrow(E_F) + N_\uparrow(E_F)}$$

where $N_\downarrow(E_F)$ and $N_\uparrow(E_F)$ are the densities of states for spin-up and spin-down electrons, respectively.

2. Spin-polarization can be probed by electron tunnelling across an insulating barrier, either using two FM electrodes or one ferromagnet and one superconductor electrode. The tunnelling spin polarization is defined by

$$P_{Tunnel} = \frac{N_\downarrow(E_F) |T_\downarrow^2| - N_\uparrow(E_F) |T_\uparrow^2|}{N_\downarrow(E_F) |T_\downarrow^2| + N_\uparrow(E_F) |T_\uparrow^2|}$$

where $T_{\uparrow,\downarrow}$ is the tunnelling matrix element.

Figure 10.2: Schematic view of a point contact in a PCAR experiment.
(3) Alternatively, the spin polarization can be measured by using PCAR technique. Andreev Reflection (AR) is a scattering process where electrical current is converted to supercurrent at an interface between a normal metal (ferromagnetic metal) and a superconductor [1]. At the interface in a metal - superconductor device, an electron incident from the metal side with energy smaller than the energy gap in the superconductor is converted into a hole which moves backward with respect to electron. The missing charge $2e$ propagates as an electron pair into the superconductor. The electron – hole conversion is known as AR. Hence, in the PCAR technique, the difference between spin-dependent currents is measured. The first intuitive and simple description of the conductance through a ballistic ferromagnet – superconductor point contact was presented by de Jong and Beenakker [1]. They consider a ferromagnetic – superconductor point contact where the ferromagnet is contacted through a small area with a superconductor, as shown in Figure 10.2. In the contact region the number of spin-up transmitting channels ($N_↑$) is larger than that of spin-down transmitting channels ($N_↓$), i.e., $N_↑ \geq N_↓$. They suppose that there is no partially transmitting channels and neglect mixing of channels for simplicity. When the superconductor is in the normal conducting state ($SC_N$), all scattering channels (transverse modes in the point contact at the Fermi level) are fully transmitted, yielding the conductance

$$G_{FM-SC_N} = \frac{e^2}{\hbar} (N_1 + N_1)$$  \hfill (10.3)

When the tip is in the superconducting state, all the spin-down incident electrons in $N_↓$ channels are Andreev reflected and give a double contribution to the conductance, $2(e^2/\hbar)(N_↓)$. However, spin-up incident electrons in some channels cannot be Andreev reflected since the density of states for spin-down electrons is smaller than that for spin-up electrons. Then only a fraction ($N_↓/N_↑$) of the $N_↑$ channels can be Andreev reflected and the resulting conductance are $2(e^2/\hbar)(N_↓/N_↑)N_↑$. The total conductance at zero bias voltage ($V = 0$) is given by the sum of these two contributions:

$$G_{FM-SC} = \frac{e^2}{\hbar} 2 \left( N_1 + \frac{N_1}{N_↑} N_↑ \right) = \frac{e^2}{\hbar} 4N_↓$$  \hfill (10.4)

Taking the ratio of eqns. (10.3) and (10.4), we obtain the normalized conductance

$$\frac{G_{FM-SC}}{G_{FM-SC_N}} = \frac{4N_↓}{(N_↑ + N_↓)} = 2(1 - P)$$  \hfill (10.5)

where $P$ is the spin polarization of the transmitting channel defined as

$$P = \frac{N_↑ - N_↓}{N_↑ + N_↓}$$  \hfill (10.6)
Eqn. (10.5) shows that the normalized conductance is a monotonic decreasing function of $P$ and it vanishes if the ferromagnet is half-metallic ($P = 1$). Depending on the degree of spin polarization only for a fraction of electrons, an electron with the opposite spin is available. Thus, a spin polarization at the Fermi energy in a ferromagnet partially or completely suppresses the AR. Hence, the current through the point contact can be divided into an unpolarized current and a polarized current.

$$I = (1 - P)I_{unpol} + P.I_{pol} \tag{10.7}$$

The fraction $(1-P)$ of the electrons are AR reflected, the remaining fraction $P$ is normally reflected. Both unpolarized current and polarized current can be calculated using eqn.(10.7). The typical variation of conductance curve for the materials with different spin polarization obtained using PCAR technique is schematically shown in Fig.10.3. A high value of $P$ reduces the zero-bias conductance peak dramatically due to the bigger fraction of the electrons that are normally reflected. This theoretical model is called ballistic model.

**References:**

**Quiz:**
(1) What is Andreev Reflections?
(2) Which type of materials exhibits high spin polarization? Why?
(3) What are the various ways of defining spin polarization?