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SPIN-DEPENDENT SCATTERING ON THE INTERFACE LAYERS IN MAGNETIC MULTI-LAYERS *

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We present a calculation of the transmission coefficients $T^{\uparrow(\downarrow)}$. The idea of the calculation of $T^{\uparrow(\downarrow)}$ is the following: Starting from the exchange Hamiltonian of the Heisenberg type which describes the exchange energy of the d-electrons in the ferromagnetic layers and the exchange interaction energy between d and s electrons, we statistically averaged the exchange interaction energy according to the distribution function of d-electrons at the given temperature and magnetic field. The average energy represents the potential discontinuities at the interface between paramagnetic and ferromagnetic layers. The scattering of the s-electrons on the potential discontinuities represents the microscopic origin of the coefficients $T^{\uparrow(\downarrow)}$. It was shown that these coefficients are angular and spin-dependent.

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1 Introduction

Magnetic multi-layers (MML) reveal a range of interesting and attractive features resulting from the interplay of electronic and magnetic properties which cannot be observed in a single film. The MML are composed of metallic layers where there is a paramagnetic layer in between two ferromagnet layers. By layering one can modify the material properties or obtain new properties, uncharacteristic for bulk materials and this was the reason for studying the MML. The study of the transport properties of these MML is very interesting because they exhibit giant magnetoresistance (GMR). The GMR was observed first on Fe-Cr-Fe layered structure in [1] and at the same time in [2]. The GMR is due to the existence of magnetic coupling between two ferromagnetic layers separated by a paramagnetic layer (spacer layer). In attempting to explain this exchange coupling, theorists have proposed a wide variety of models, in many cases drawing on earlier works. Many of the models proposed for exchange coupling between two ferromagnet (FM) layers through a paramagnet (PM) layer are based on the model of coupling between magnetic impurities in the host metal. The most widely applied one of these early models is Ruderman-Kittel-Kasuya-Yosida (RKKY) coupling [3–5]. The magnetization of neighbouring FM layers can be parallel (ferromagnetic alignment F) or anti-parallel (anti-ferromagnetic alignment AF). The character of the exchange coupling (F or AF) depends on the thickness of the spacer layer and with an increase of the thickness it oscillates with a certain period. The short-period oscillations in the interlayer exchange coupling in Fe-Cr-Fe have been attributed to an

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RKKY-type interaction through paramagnetic Cr [6]. Evidence has been found for two periods of oscillations in Fe-Cr-Fe(001) [7] and [8]. Two periods of oscillations have also been found in Co-Cu-Co(001) [9] and Fe-Ag-Fe(001) [10–12] and [13]. Additionally, short period oscillations in the magnetic coupling have been observed for Fe-Cu-Fe(001) [9]. If the exchange coupling is AF, then by applying a strong enough magnetic field in the layer plane the AF coupling may be overcome and the magnetic moments of all FM layers can be forced to be oriented in the same direction. Experimentally it has been observed that the resistance decreases when the layer magnetization rotates from AF alignment to the F one. The GMR is defined by the formula

$$GMR = \frac{\rho_{\uparrow\downarrow} - \rho_{\downarrow\downarrow}}{\rho_{\downarrow\downarrow}}$$

where $\rho_{\uparrow\downarrow}$ is the resistivity in AF alignment, $\rho_{\downarrow\downarrow}$ is the resistivity in F alignment.

The magnetoresistance effect increases by about a factor of $2 \div 3$ when the temperature changes from room temperature to that of liquid He. Experimentally it has been shown that the large magnetoresistance effect in layered structures is nearly the same for current flowing parallel or perpendicular to the magnetizations and the small difference can be attributed to the magnetoresistivity anisotropy effect.

The large magnetoresistance effect is also observed in granular alloys where the ferromagnetic granules are embedded in a nonmagnetic matrix [14, 15] and [16]. The approach to the theoretical description of the magnetoresistance in MML may be based either on a semiclassical model or on a quantum one. The semiclassical model was worked out first by Camley and Barnas [17] and [18]. The semiclassical model is an extension of the Fuchs-Sondheimer semiclassical model for the conduction in thin films [19] and [20] to the case of MML. The model of Camley and Barnas has been extensively used for numerical calculations of the GMR in sandwiches and multilayers [21].

The quantum approach to the GMR has been worked out by Levy et al. [22]. This approach is based on the Kubo-Greenwood formula, which is used to treat the scattering of electron waves (free electrons) by spin dependent potential randomly distributed in the interface planes or within the layers (spin dependence scattering only within the FM layers). The quantum models have been extensively used also for numerical calculations of the GMR [23–26] and [27].

Now we focus our attention to the semiclassical approach to the GMR in MML because the testing of the results of the semiclassical theory by comparing them with the experimental one is quite good. Using the same procedure as in [18] we can write the Boltzmann transport equation

$$\frac{\partial g^{\uparrow(\downarrow)}(z,\mathbf{v})}{\partial z} + \frac{g^{\uparrow(\downarrow)}(z,\mathbf{v})}{\tau^{\uparrow(\downarrow)} v_z} = \frac{eE}{m v_z} \frac{\partial f^{(0)}(\mathbf{v})}{\partial v_x}, \tag{1}$$

where e ($e > 0$) and m denote the electron charge and electron effective mass (assumed independent of electron spin), $\tau^{\uparrow(\downarrow)}$ are the relaxation times for spin-up and spin-down electrons, E is the electric field, which is parallel to x-axis. x-axis is parallel and z-axis is perpendicular to the layer plane. In each layer the electric current is determined by the appropriate distribution function $f^{\uparrow(\downarrow)}(z,\mathbf{v})$ for electrons with spin-up and spin-down and with the velocity $\mathbf{v}$. The distribution function $f^{\uparrow(\downarrow)}(z,\mathbf{v})$ is decomposed into two parts: the equilibrium distribution function $f^{(0)}(\mathbf{v})$ and small contribution $g^{\uparrow(\downarrow)}(z,\mathbf{v})$ induced by the external field. The general solution of equation (1) can be written in the form

$$g_{\pm}^{\uparrow(\downarrow)}(z,\mathbf{v}) = \frac{eE\tau^{\uparrow(\downarrow)}}{m}\frac{\partial f^{(0)}(\mathbf{v})}{\partial v_x}\left\{1 + F_{\pm}^{\uparrow(\downarrow)}(\mathbf{v})\exp\left[\frac{\pm z}{\tau^{\uparrow(\downarrow)}|v_y|}\right]\right\}, \tag{2}$$

where $+$ and $-$ are for $v_z > 0$ and $v_z < 0$, respectively. The unknown functions $F_{\pm}^{\uparrow(\downarrow)}(\mathbf{v})$ are determined from the boundary conditions. There are four Fuchs boundary conditions at the free surfaces:

$$g_{+}^{\uparrow(\downarrow)}(z=0,\mathbf{v}) = p^{\uparrow(\downarrow)}(z=0)g_{-}^{\uparrow(\downarrow)} \tag{3}$$

$$g_{-}^{\uparrow(\downarrow)}(z=d,\mathbf{v}) = p^{\uparrow(\downarrow)}(z=d)g_{+}^{\uparrow(\downarrow)}, \tag{4}$$

where $p^{\uparrow(\downarrow)}(z=0)$ and $p^{\uparrow(\downarrow)}(z=d)$ are the Fuchs specularity factors.
Boundary conditions at the interface $z = d_i$:

$$g_{-}^{\uparrow(\downarrow)}(z=d_i^{-},\mathbf{v}) = T^{\uparrow(\downarrow)}g_{-}^{\uparrow(\downarrow)}(z=d_i^{+},\mathbf{v}) + R^{\uparrow(\downarrow)}g_{+}^{\uparrow(\downarrow)}(z=d_i^{-},\mathbf{v}) \tag{5}$$

$$g_{+}^{\uparrow(\downarrow)}(z=d_i^{+},\mathbf{v}) = T^{\uparrow(\downarrow)}g_{+}^{\uparrow(\downarrow)}(z=d_i^{-},\mathbf{v}) + R^{\uparrow(\downarrow)}g_{-}^{\uparrow(\downarrow)}(z=d_i^{+},\mathbf{v}), \tag{6}$$

where $T^{\uparrow(\downarrow)}$ and $R^{\uparrow(\downarrow)}$ are the non-diffusive (specular) transmission and reflection coefficients at the interface between neighbouring layers. In [18] there was neglected any angular dependence of these coefficients and the same transmission and reflection coefficients for electrons incident on interface from the left and right sides were assumed.

If we have n layers, then there are $4n$ unknown functions of the $F_{\pm}^{\uparrow(\downarrow)}$ type. At the free surfaces there are four boundary conditions. At interface layers we have $4(n-1)$ boundary conditions of the type (5) and (6). Together we have $4 + 4(n-1) = 4n$ boundary conditions and this is enough for the determination of all unknown functions of the $F_{\pm}^{\uparrow(\downarrow)}$ type.

We suppose that the spin dependent interface scattering may play an essential role in GMR, and therefore the main aim of this papers is to determine the origin of the transmission and reflection coefficients.

Before we start to solve the problem of the origin of $T^{\uparrow(\downarrow)}$ and $R^{\uparrow(\downarrow)}$, we summarize the experimental facts which were the motivation for this paper. By summarizing some experimental data we come to the following conclusions:

1. The existence of GMR is promising for applications in magneto-resistance sensors.
2. GMR can arise from two different mechanisms: spin-dependent bulk scattering anisotropy ($\tau^{\uparrow} \neq \tau^{\downarrow}$) and spin-dependent interface scattering anisotropy ($T^{\uparrow} \neq T^{\downarrow}$).
3. Significant effect on the resistivity of the MML is expected only for scattering by interface roughness.
4. The spin-flips scattering in the spacer layers suppresses the GMR arising from both the bulk and surface scattering anisotropies of the spin-up and spin-down electrons [21].
5. The spin-flip scattering in ferromagnetic layers selectively suppresses the bulk-scattering anisotropy and enhances the relative role of the surface-scattering anisotropy [21].

2 Theoretical model of spin-dependent scattering on the interface layers in MML

2.1 Hamiltonian of $d - s$ electrons

As it was mentioned in the introduction, one of the methods of the theoretical description the transport properties of the magnetoresistance in MML is the semiclassical model which is an extension of the Fuchs-Sondheimer model for the conduction in thin films to the case of MML. This semiclassical approach needs to known the transmission coefficients $T^{\uparrow(\downarrow)}$ at the interface between neighbouring layers. Nevertheless, the major open problem is still the microscopic origin of the spin dependent scattering by interfaces, i.e, the problem of the microscopic mechanism giving rise to different values of $T^{\uparrow}$ and $T^{\downarrow}$. For this reason the main aim of this paper is to show the microscopic origin of these coefficients. For this purpose let us consider the Hamiltonian of the d and s electrons of the MML as

$$\hat{H} = \hat{H}_d + \hat{H}_s + \hat{H}_{d-s} , \tag{7}$$

where

$$\hat{H}_d = -\sum_i \frac{\hbar^2}{2m} \triangle_i + \sum_i \sum_{j,j\neq i} \frac{e^2}{4\pi\varepsilon_0} \frac{1}{|\mathbf{r}_{di} - \mathbf{r}_{dj}|} \tag{8}$$

is the Hamiltonian of the d-electrons in ferromagnetic layers,

$$\hat{H}_s = -\sum_l \frac{\hbar^2}{2m} \triangle_l + \sum_l \sum_{n,n\neq l} \frac{e^2}{4\pi\varepsilon_0} \frac{1}{|\mathbf{r}_{sl} - \mathbf{r}_{sn}|} \tag{9}$$

is the Hamiltonian of s-electrons in both paramagnetic and ferromagnetic layers,

$$\hat{H}_{d-s} = \sum_i \sum_l \frac{e^2}{4\pi\varepsilon_0} \frac{1}{|\mathbf{r}_{di} - \mathbf{r}_{sl}|} \tag{10}$$

is the interaction Hamiltonian of d and s electrons. There is no doubt that the s-electrons in both types of layers are conduction ones. For this reason one can use the one electron approximation in which the quantum state of the s-electron is described by Bloch's function. This cannot be said about the d-electrons in the transition metals. The large value of the electronic part of the specific heat capacity is interpreted with the conception that some part of the d-electrons are localized and others are delocalized. Until now, this problem has not been resolved satisfactorily. Nevertheles, we will use the results of [28, 29] and [30], where the authors started from the general many-body Hamiltonian and treated $\hat{H}_{s-d}$ up to the second order in perturbation theory. In this approximation the exchange part of the Hamiltonian can be written in the following form

$$\hat{H}_{ex} = \hat{H}_d + \hat{H}_{sd} , \tag{11}$$

where

$$\hat{H}_d = -\sum_{\mathbf{R}_n} \sum_{\mathbf{R}_{m,m\neq n}} I(|\mathbf{R}_n - \mathbf{R}_m|)\hat{\mathbf{S}}(\mathbf{R}_n).\hat{\mathbf{S}}(\mathbf{R}_m), \tag{12}$$

$$\hat{H}_{sd} = -\sum_{n\mathbf{k}}\sum_{\mathbf{R}_n} \tilde{I}_n \hat{\mathbf{S}}(\mathbf{R}_n).\hat{\mathbf{S}}_{n\mathbf{k}}, \tag{13}$$

$\{\hat{\mathbf{S}}(\mathbf{R}_n)\}$ are the spin angular momentum operators (in units of $\hbar$) of d-electrons of the atom at the place $\mathbf{R}_n$ in the ferromagnetic layer,

$\hat{\mathbf{S}}_{n\mathbf{k}}$ is the spin angular momentum operator (in units of $\hbar$) of the electron in the n-band and in the quantum state determined by the $\mathbf{k}$,

$\{\mathbf{R}_n\}$ and $\{\mathbf{R}_m\}$ are the vectors in Bravais lattice,

$I(|\mathbf{r}_n - \mathbf{R}_m|)$ are the exchange integrals which are assumed to be positive,

$\tilde{I}_n$ is the exchange integral between d and s electrons. The $\tilde{I}_n$ do not depend on the wave vector $\mathbf{k}$.

For the calculation of the transmission coefficient it is sufficient to consider only one s electron. In the double sum in (12) it is sufficient to consider only the nearest neighbours. Considering this fact the exchange Hamiltonian of the Heisenberg type [31] in the external field can be written in the following form

$$\hat{H}_{ex} = -I\sum_{\mathbf{R}_n}\sum_{\mathbf{R}_{m,m\neq n}} \hat{\mathbf{S}}(\mathbf{R}_n).\hat{\mathbf{S}}(\mathbf{R}_m) - \tilde{I}_n\sum_{\mathbf{R}_n}\hat{\mathbf{S}}(\mathbf{R}_n).\hat{\mathbf{S}}_{n\mathbf{k}} - \sum_{\mathbf{R}_n}\hat{\mathbf{m}}(\mathbf{R}_n).\mathbf{H} - \hat{\mathbf{m}}_{n\mathbf{k}}.\mathbf{H}\,, \tag{14}$$

where vectors $\{\mathbf{R}_m\}$ are the position vectors of the nearest neighbours of the atom at the place $\mathbf{R}_n$ in Bravais lattice,

$$\hat{\mathbf{m}}(\mathbf{R}_n) = -g\mu_B\hat{\mathbf{S}}(\mathbf{R}_n) \tag{15}$$

is the magnetic moment operator of the d-electrons belonging to the atom at the place $\mathbf{R}_n$ in the Bravais lattice,

$$\hat{\mathbf{m}}_{n\mathbf{k}} = -2\mu_B\hat{\mathbf{S}}_{n\mathbf{k}} \tag{16}$$

is the magnetic moment operator of the $n\mathbf{k}$-electron, $\mu_B = \frac{1}{2}\frac{|e|\mu_0\hbar}{m_0}$ is the Bohr magneton, g is the Landé factor.

The idea of the calculation of $T^{\uparrow(\downarrow)}$ will be the following: At first we will calculate the statistical average of the interaction energy between d-electrons and one $n\mathbf{k}$ electron

$$W_n = -\langle\sum_{\mathbf{R}_n}\tilde{I}_n\hat{\mathbf{S}}(\mathbf{R}_n).\hat{\mathbf{S}}_{n\mathbf{k}}\rangle\,. \tag{17}$$

When we know the W_n, then we can use the well-known formula for the calculation of the $T^{\uparrow(\downarrow)}$.

2.2 Low temperatures

For the averaging procedure we have to know the elementary exitation quantum states of the $\hat{H}_d$. But this can be done analytically only for low and high temperatures. As mentioned in the introduction, the GMR increases when the temperature changes from room temperature to that one of liquid He. This is the second reason why we are interested in the spin-dependent scattering on the interface layer at sufficiently low temperatures. In this case it is more convenient to transform the exchange Hamiltonian to the boson creation and annihilation operators $\hat{a}^+(\mathbf{R}_n)$,

$\hat{a}(\mathbf{R}_n)$ by the Holstein-Primakoff transformation [32]. The transformation is defined by the relations

$$\hat{S}^{+}(\mathbf{R}_n) = \hat{S}_x(\mathbf{R}_n) + i\hat{S}_y(\mathbf{R}_n) = (2S)^{\frac{1}{2}}\sqrt{1 - \frac{\hat{a}^{+}(\mathbf{R}_n)\hat{a}(\mathbf{R}_n)}{2S}}\hat{a}(\mathbf{R}_n)\,, \tag{18}$$

$$\hat{S}^{-}(\mathbf{R}_n) = \hat{S}_x(\mathbf{R}_n) - i\hat{S}_y(\mathbf{R}_n) = (2S)^{\frac{1}{2}}\hat{a}^{+}(\mathbf{R}_n)\sqrt{1 - \frac{\hat{a}^{+}(\mathbf{R}_n)\hat{a}(\mathbf{R}_n)}{2S}}\,, \tag{19}$$

$$\hat{S}_z(\mathbf{R}_n) = SI - \hat{a}^{+}(\mathbf{R}_n)\hat{a}(\mathbf{R}_n)\,. \tag{20}$$

The creation and annihilation operators $\hat{a}^{+}(\mathbf{R}_n)$ and $\hat{a}(\mathbf{R}_n)$ fulfill the commutation relation

$$[\hat{a}^{+}(\mathbf{R}_n), \hat{a}(\mathbf{R}_m)] = \delta_{\mathbf{R}_n,\mathbf{R}_m}\,. \tag{21}$$

At sufficiently low temperature it is enough to be concerned mainly with low-lying states of the system of d electrons such that the fractional spin reversal is small:

$$\frac{\langle \hat{a}^{+}(\mathbf{R}_n)\hat{a}(\mathbf{R}_n)\rangle}{S} = \frac{\langle \hat{n}(\mathbf{R}_n)\rangle}{S} \ll 1\,,$$

where $\langle \hat{n} \rangle$ is the average number of electrons at the place $\mathbf{R}_n$. Then we can expand the square roots in (18) and (19):

$$\sqrt{1 - \frac{\hat{a}^{+}(\mathbf{R}_n)\hat{a}(\mathbf{R}_n)}{2S}} \approx 1 - \frac{\hat{a}^{+}(\mathbf{R}_n)\hat{a}(\mathbf{R}_n)}{4S} + ... \tag{22}$$

Introducing (22) into (18) and (19) one obtains

$$\hat{S}^{+}(\mathbf{R}_n) = (2S)^{\frac{1}{2}}\left[\hat{a}(\mathbf{R}_n) - \frac{\hat{a}^{+}(\mathbf{r}_n)\hat{a}(\mathbf{R}_n)\hat{a}(\mathbf{R}_n)}{4S} + ...\right] \tag{23}$$

$$\hat{S}^{-}(\mathbf{R}_n) = (2S)^{\frac{1}{2}}\left[\hat{a}^{+}(\mathbf{R}_n) - \frac{\hat{a}^{+}(\mathbf{R}_n)\hat{a}^{+}(\mathbf{R}_n)\hat{a}(\mathbf{R}_n)}{4S} + ...\right]\,. \tag{24}$$

In this case we choose z-axis parallel to the layer plane and we will assume that the spin angular momentum $\hat{\mathbf{S}}_{n\mathbf{k}}$ has only z-component. The Hamiltonian (14) has the following form

$$\begin{aligned} \hat{H}_{ex} \quad = \quad & -I\sum_{\mathbf{R}_n}\sum_{\mathbf{R}_m}\hat{\mathbf{S}}(\mathbf{R}_n).\hat{\mathbf{S}}(\mathbf{R}_m) - \tilde{I}_n\sum_{\mathbf{R}_n}\hat{S}_z(\mathbf{R}_n)\hat{S}_{n\mathbf{k}z} - g\mu_B\sum_{\mathbf{R}_n}\hat{S}_z(\mathbf{R}_n)H - \\ & -2\mu_B\hat{S}_{n\mathbf{k}z}H, \end{aligned} \tag{25}$$

where we consider that $\mathbf{H} = -H\mathbf{e}_3$ ($H > 0$). The unit vector $\mathbf{e}_3$ is parallel to the z-axis. At temperature $T = 0$K we will assume that the z component of the spin angular momentum of all d electrons has direction up, so the magnetization $\mathbf{M} = -M\mathbf{e}_3$ ($M > 0$). This is the reason why we chose the magnetic field in the same direction as the $\mathbf{M}$. In the opposite case the system of d electrons would be thermodynamically unstable at the large value of H.

It may be convenient to make a transformation from the atomic operators $\hat{a}^{+}(\mathbf{R}_n)$, $\hat{a}(\mathbf{R}_n)$ to the magnon variables $\hat{b}^{+}_{\mathbf{q}}$ and $\hat{a}_{\mathbf{q}}$ defined by

$$\hat{b}_{\mathbf{q}} = \frac{1}{\sqrt{N}} \sum_{\mathbf{R}_n} e^{i\mathbf{q}.\mathbf{R}_n} \hat{a}(\mathbf{R}_n) \,, \tag{26}$$

$$\hat{b}^{+}_{\mathbf{q}} = \frac{1}{\sqrt{N}} \sum_{\mathbf{R}_n} e^{-i\mathbf{q}.\mathbf{R}_n} \hat{a}^{+}(\mathbf{R}_n) \,. \tag{27}$$

Introducing (23), (24), (26) and (27) into (25) one obtains

$$\hat{H}_{ex} = -INzS^2 - \tilde{I}_n NS\hat{S}_{n\mathbf{k}z} - g\mu_B NSH + \hat{H}_0 + \hat{H}_{int} \,, \tag{28}$$

where z is the number of neighbouring atoms to the atom at the place $\mathbf{R}_n$ in the Bravais lattice,

$$\begin{aligned} \hat{H}_0 \quad = \quad & -IzS \sum_{\mathbf{q}} \{\gamma_{\mathbf{q}} \hat{b}_{\mathbf{q}} \hat{b}^{+}_{\mathbf{q}} + \gamma_{-\mathbf{q}} \hat{b}^{+}_{\mathbf{q}} \hat{b}_{\mathbf{q}} - 2\hat{b}^{+}_{\mathbf{q}} \hat{b}_{\mathbf{q}}\} + g\mu_B H \sum_{\mathbf{q}} \hat{b}^{+}_{\mathbf{q}} \hat{b}_{\mathbf{q}} + \\ & + \tilde{I}_n \sum_{\mathbf{q}} \hat{b}^{+}_{\mathbf{q}} \hat{b}_{\mathbf{q}} \hat{S}_{n\mathbf{k}z} - 2\mu_B H \hat{S}_{n\mathbf{k}z} \,, \end{aligned} \tag{29}$$

where $\gamma_{\mathbf{q}} = \frac{1}{z} \sum_{\mathbf{a}_i} e^{i\mathbf{q}.\mathbf{a}_i}$. Vectors $\mathbf{a}_i$ connect the atom at the place $\mathbf{R}_n$ with its nearest neighbours in the Bravais lattice.

$\hat{H}_{int}$ contains fourth and higher order terms in magnons operators, and it may be neglected when the excitation is low. We note that $\sum_{\mathbf{q}} \gamma_{\mathbf{q}} = 0$.

If there is a center of symmetry $\gamma_{\mathbf{q}} = \gamma_{-\mathbf{q}}$, then

$$\hat{H}_0 = \sum_{\mathbf{q}} \{2IzS(1-\gamma_{\mathbf{q}}) + g\mu_B H + \tilde{I}_n \hat{S}_{n\mathbf{k}z}\} \hat{b}^{+}_{\mathbf{q}} \hat{b}_{\mathbf{q}} - 2\mu_B H \hat{S}_{n\mathbf{k}z} \,. \tag{30}$$

For a body-centered cubic lattice we can write

$$z(1-\gamma_{\mathbf{q}}) = 8 - 8\cos\frac{a}{2}q_x \cos\frac{a}{2}q_y \cos\frac{a}{2}q_z \,. \tag{31}$$

Near to the bottom of the magnon band ($q_x a \ll 1$, $q_y a \ll 1$ and $q_z a \ll 1$) relation (31) can be written in the form

$$z(1-\gamma_{\mathbf{q}}) \approx a^2(q_x^2 + q_y^2 + q_z^2) \,. \tag{32}$$

Introducing (32) into (30) we obtain

$$\hat{H}_0 = \sum_{\mathbf{q}} \hat{n}_{\mathbf{q}} \omega_{\mathbf{q}} - 2\mu_B H \hat{S}_{n\mathbf{k}z} \,, \tag{33}$$

where

$$\begin{aligned} \omega_{\mathbf{q}} \quad = \quad & 2IzS(1-\gamma_{\mathbf{q}}) + g\mu_B H + \tilde{I}_n \hat{S}_{n\mathbf{k}z} \approx 2SIa^2(q_x^2 + q_y^2 + q_z^2) + g\mu_B H + \\ & + \tilde{I}_n \hat{S}_{n\mathbf{k}z} = \frac{\hbar^2}{2m^*}(q_x^2 + q_y^2 + q_z^2) + g\mu_B H + \tilde{I}_n \hat{S}_{n\mathbf{k}z}, \end{aligned} \tag{34}$$

$\frac{\hbar^2}{2m^*} = 2SIa^2$, m^* is the effective mass, $\hat{n}_{\mathbf{q}} = \hat{b}^+_{\mathbf{q}}\hat{b}_{\mathbf{q}}$ is the number of magnons with wavevector $\mathbf{q}$.

The interaction energy between d and s electrons is expressed by the relation

$$\tilde{I}_n(\hat{n}_{\mathbf{q}} - NS)\hat{S}_{n\mathbf{k}z}\,, \tag{35}$$

where the eigenvalues of $\hat{S}_{n\mathbf{k}z}$ are $\pm\frac{1}{2}$. We see that the interaction energy between d and s electrons is spin-dependent.

2.3 High temperatures

It woud be very good to know how the GMR changes continuously with temperature. But as it was mentioned, one can determine analytically only the average energy W_n only in extreme cases, i.e. at low and high temperatures. In this case we will use the mean field approximation. From relation (15) we calculate $\hat{S}(\mathbf{R}_n)$ and introduce it in (14). After introducing we obtain

$$\begin{aligned}\hat{H}_{ex} &= -\frac{I}{(g\mu_B)^2}\sum_{\mathbf{R}_n}\sum_{\mathbf{R}_m}\hat{\mathbf{m}}(\mathbf{R}_n).\hat{\mathbf{m}}(\mathbf{R}_m) + \frac{\tilde{I}_n}{g\mu_B}\sum_{\mathbf{R}_n}\hat{\mathbf{m}}(\mathbf{R}_n).\hat{\mathbf{S}}_{n\mathbf{k}} \\ &\quad - \sum_{\mathbf{R}_n}\hat{\mathbf{m}}(\mathbf{R}_n).\mathbf{H} - \hat{\mathbf{m}}_{n\mathbf{k}}.\mathbf{H}\,.\end{aligned} \tag{36}$$

In the framework of the mean field approximation we substitute $\hat{\mathbf{m}}(\mathbf{R}_n)$ in (36) by $\langle\hat{\mathbf{m}}(\mathbf{R}_m)\rangle$. Due to the translation symmetry we can write

$$\mathbf{M} = N_0\langle\hat{\mathbf{m}}(\mathbf{R}_n)\rangle\,, \tag{37}$$

where $\mathbf{M}$ is the magnetization, N_0 is the number of atoms in the unit volume.
Introducing (37) into (36) one obtains

$$\hat{H}_{ex} = -\sum_{\mathbf{R}_n}\hat{\mathbf{m}}(\mathbf{R}_n).[b\mathbf{M} + \mathbf{H} - \frac{\tilde{I}_n}{g\mu_B}\hat{\mathbf{S}}_{nk}] - \hat{\mathbf{m}}_{nk}.\mathbf{H}\,, \tag{38}$$

where $b = \frac{zI}{N_0(g\mu_B)^2}$.
According to (38) the interaction energy between d and s electrons is expressed by the term

$$\sum_{\mathbf{R}_n}\hat{\mathbf{m}}(\mathbf{R}_n).\frac{\tilde{I}_n}{g\mu_B}.\hat{\mathbf{S}}_{n\mathbf{k}}\,. \tag{39}$$

We see again that the interaction energy between d and s electrons is spin dependent.

3 Average interaction energy between d and s electrons

3.1 Low temperatures

According to (28) and (29) the average interaction energy between d and s electrons is expressed by the relation

$$W_n = \tilde{I}_n\left(\sum_{\mathbf{q}}\langle\hat{n}_{\mathbf{q}}\rangle - NS\right)\hat{S}_{n\mathbf{k}z}\,, \tag{40}$$

where $\langle\rangle$ means the statistical average value at the given temperature. The averaging at the given temperature is defined by the Gibbs canonical distribution function

$$w_{\mathbf{q}} = \frac{e^{-\beta n_{\mathbf{q}}\varepsilon_{\mathbf{q}}}}{Z}\,, \tag{41}$$

where $w_{\mathbf{q}}$ is the probability that the system of d electrons has the excitation energy $n_{\mathbf{q}}\varepsilon_{\mathbf{q}}$,

$$\varepsilon_{\mathbf{q}} = \frac{\hbar^2}{2m^*}(q_x^2 + q_y^2 + q_z^2) + g\mu_B H, \tag{42}$$

Z is the statistical summ and $\beta = \frac{1}{k_B T}$.
The average value is defined by the relation

$$\langle n_{\mathbf{q}}\rangle = \sum_{n_{\mathbf{q}}=0}^{\infty} w_{\mathbf{q}} n_{\mathbf{q}}\,. \tag{43}$$

Using (41) and (43) one can write

$$\langle n_{\mathbf{q}}\rangle = \frac{1}{e^{\beta\varepsilon_{\mathbf{q}}} - 1}\,. \tag{44}$$

Substituting (44) into (40) we obtain

$$W_n = \tilde{I}_n \left(\sum_{\mathbf{q}} \frac{1}{e^{\beta\varepsilon_{\mathbf{q}}} - 1} - NS\right) \hat{S}_{n\mathbf{k}z}\,. \tag{45}$$

Considering the periodic boundary conditions, then $q_x = \frac{2\pi}{aN_1}n_1$, $q_y = \frac{2\pi}{aN_2}n_2$, and $q_z = \frac{2\pi}{aN_3}n_3$. According to relation (44) and the periodic boundary conditions we can write

$$\begin{aligned} \sum_{\mathbf{q}} \frac{1}{e^{\beta\varepsilon_{\mathbf{q}}} - 1} &\approx \int dn_1 \int dn_2 \int dn_3 \frac{1}{e^{\beta\varepsilon_{\mathbf{q}}} - 1} = \\ &= 2\pi V \left(\frac{2m^* k_B T}{h^2}\right)^{\frac{3}{2}} \int_0^{\infty} \frac{\sqrt{x}dx}{e^{x+\beta g\mu_B H} - 1}\,. \end{aligned} \tag{46}$$

Multiplying (45) by $g\mu_B$ we obtain

$$g\mu_B W_n = \tilde{I}_n \left(g\mu_B \sum_{\mathbf{q}} \frac{1}{e^{\beta\varepsilon_{\mathbf{q}}} - 1} - VM_0\right) \hat{S}_{n\mathbf{k}z}\,, \tag{47}$$

where M_0 is the magnetization at temperature $T = 0\,\mathrm{K}$.

Magnetization of the d electrons is expressed by the relation

$$\begin{aligned} VM &= g\mu_B S(n^{\uparrow} - n^{\downarrow}) = g\mu_B S(N - 2n^{\downarrow}) = \\ &= g\mu_B S\left(N - 2\sum_{\mathbf{q}} \frac{1}{e^{\beta\varepsilon_{\mathbf{q}}} - 1}\right) = VM_0 - 2g\mu_B S \sum_{\mathbf{q}} \frac{1}{e^{\beta\varepsilon_{\mathbf{q}}} - 1}\,, \end{aligned} \tag{48}$$

where $n^{\uparrow}$ is the number of atoms with spin-up and $n^{\downarrow}$ is the number of atoms with spin-down. We calculate M_0 from (48) and substitute it into (47). Doing this we obtain

$$g\mu_B W_n = \tilde{I}_n \left[VM + (2S-1) g\mu_B \sum_{\mathbf{q}} \frac{1}{e^{\beta\varepsilon_{\mathbf{q}}} - 1} \right] \hat{S}_{\mathbf{nk}z} \,. \tag{49}$$

After introducing (46) into (48) we obtain

$$W_n = -\tilde{I}_n \left[VM + (2S-1) g\mu_B 2\pi V \left(\frac{2m^* k_B T}{h^2} \right)^{\frac{3}{2}} \int_0^{\infty} \frac{\sqrt{x}dx}{e^{x+\beta g\mu_B H} - 1} \right] \hat{S}_{\mathbf{nk}z} \,. \tag{50}$$

What is the sign of the W_n that depends on the sign of the exchange integral $\tilde{I}_n$. In the case when the $\tilde{I}_n$ is positive then for $S_{n\mathbf{k}z} = \frac{1}{2}$, $W_n < 0$ and for $S_{n\mathbf{k}z} = -\frac{1}{2}$, $W_n > 0$. In the case when the $\tilde{I}_n$ is negative then for $S_{n\mathbf{k}z} = \frac{1}{2}$, $W_n > 0$ and for $S_{n\mathbf{k}z} = -\frac{1}{2}$, $W_n < 0$. This is the original result.

3.2 High temperature

In this case the average interaction energy of d and s electrons according to relation (39) is expressed by the relation

$$W_n = \sum_{\mathbf{R}_n} \langle \hat{\mathbf{m}}(\mathbf{R}_n) \rangle . \frac{\tilde{I}_n}{g\mu_B} \hat{\mathbf{S}}_{n\mathbf{k}} \,. \tag{51}$$

Substituting relation (37) into (51) one obtains

$$W_n = \sum_{\mathbf{R}_n} \frac{\mathbf{M}}{N_0} . \frac{\tilde{I}_n}{g\mu_B} \hat{\mathbf{S}}_s = -\frac{N}{N_0} \frac{\tilde{I}_n}{g\mu_B} M \hat{S}_{n\mathbf{k}z} \tag{52}$$

because $\hat{\mathbf{S}}_{n\mathbf{k}} = \hat{S}_{sz}\mathbf{e}_3$ and $\mathbf{M} = -M\mathbf{e}_3$. If $\tilde{I}_n$ is positive then for $S_{n\mathbf{k}z} = \frac{1}{2}$, $W_n < 0$ and for $S_{n\mathbf{k}z} = -\frac{1}{2}$, $W_n > 0$. But if $\tilde{I}_n$ is negative then for $S_{n\mathbf{k}z} = \frac{1}{2}$, $W_n > 0$ and for $S_{n\mathbf{k}z} = -\frac{1}{2}$, $W_n < 0$. The same results we obtained in the part 3.1. If we know the interaction energy W_n, we can calculate the transmission coefficient $T^{\uparrow(\downarrow)}$ and the reflection $R^{\uparrow(\downarrow)}$ one. In this case of the perfect interface layer the $T^{\uparrow(\downarrow)}$ and $R^{\uparrow(\downarrow)}$ can be easily calculated. This calculation is done in many textbooks of quantum mechanics and, therefore we briefly denote the procedure of the calculation of $T^{\uparrow(\downarrow)}$. For this aim we will consider that the electron goes from the spacer layer to the ferromagnetic one. At the interface layer we can use Snell' law:

$$\begin{aligned} \theta_i &= \theta_r \\ \frac{\sin\theta_t}{\sin\theta_i} &= \frac{\sqrt{m_1 E_i}}{\sqrt{m_2(E_t - W_n)}} \,, \end{aligned} \tag{53}$$

where θ_i is the angle of incidence, θ_r is the angle of reflection, θ_t is the angle of transmission, $E_i = \frac{\hbar^2}{2m_1}(k_{xi}^2 + k_{yi}^2 + k_{zi}^2)$ is the energy of the incident electron, $E_t = \frac{\hbar^2}{2m_2}(k_{xi}^2 + k_{yi}^2 + k_{zi}^2)$ is the energy of the transmitted electron, m_1 and m_2 are the effective masses of the electrons. In the case of MML the effective masses in paramagnetic and ferromagnetic layers are equal. In the ferromagnetic layers the energy of electron in the n band is expressed by the relation

$$E_n(\mathbf{k}) = \frac{\hbar^2}{2m}(k_x^2 + k_y^2 + k_z^2) + 2\mu_B S_{n\mathbf{k}z} H + W_n \,. \tag{54}$$

According to (54) the density of states in the n-band is expressed by the relation

$$g_n(E_n(\mathbf{k})) = 2\pi V \left(\frac{2m}{h^2}\right)^{\frac{3}{2}} \sqrt{E_n(\mathbf{k}) - 2\mu_B S_{n\mathbf{k}z} H - W_n}\,. \tag{55}$$

Relations (54) and (55) one can apply to the different cases:

1. $\tilde{I}_n > 0$
   - $S_{nz} = \frac{1}{2}$

     $$g_n(E_n(\mathbf{k})) = 2\pi V \left(\frac{2m}{h^2}\right)^{\frac{3}{2}} \sqrt{E_n(\mathbf{k}) - 2\mu_B S_{n\mathbf{k}z} H + |W_n|} \tag{56}$$

     and

     $$E_{n,min} = E_n(0) = 2\mu_B S_{n\mathbf{k}z} H - |W_n| \tag{57}$$

   - $S_{nz} = -\frac{1}{2}$

     $$g_n(E_n(\mathbf{k})) = 2\pi V \left(\frac{2m}{h^2}\right)^{\frac{3}{2}} \sqrt{E_n(\mathbf{k}) - 2\mu_B S_{n\mathbf{k}z} H - |W_n|} \tag{58}$$

     $$E_{n,min} = E_n(0) = 2\mu_B S_{n\mathbf{k}z} H + |W_n| \,. \tag{59}$$

   Relations (56) and (58) determine the density of states of the majority spin and the minority spin electrons, respectively. Relations (57) and (59) determine the minimum energies in the majority spin and the minority spin bands, respectively.

2. $\tilde{I}_n < 0$
   - $S_{nz} = \frac{1}{2}$

     $$g_n(E_n(\mathbf{k})) = 2\pi V \left(\frac{2m}{h^2}\right)^{\frac{3}{2}} \sqrt{E_n(\mathbf{k}) - 2\mu_B S_{n\mathbf{k}z} H - |W_n|} \tag{60}$$

     $$E_{n,min} = E_n(0) = 2\mu_B S_{n\mathbf{k}z} H + |W_n| \tag{61}$$

   - $S_{nz} = -\frac{1}{2}$

     $$g_n(E_n(\mathbf{k})) = 2\pi V \left(\frac{2m}{h^2}\right)^{\frac{3}{2}} \sqrt{E_n(\mathbf{k}) - 2\mu_B S_{n\mathbf{k}z} H + |W_n|} \tag{62}$$

     $$E_{n,min} = E_n(0) = 2\mu_B S_{n\mathbf{k}z} H - |W_n| \,. \tag{63}$$

Relations (60) and (62) determine the density of states of the minority spin and the majority spin electrons, respectively. Relations (61) and (63) determine the minimum energy in the minority spin and the majority spin bands, respectively.
Now we will proceed in the determination of the $T^{\uparrow(\downarrow)}$ After some calculations we can obtain the following relations

$$T^{\uparrow(\downarrow)} = \frac{m_1}{m_2}\frac{k_{xt}}{k_{xi}}(t^{\uparrow(\downarrow)})^2 \,,$$

$$R^{\uparrow(\downarrow)} = (r^{\uparrow(\downarrow)})^2 \,, \tag{64}$$

where

$$t^{\uparrow(\downarrow)} = \frac{2\sqrt{\frac{E}{m_1}}\cos\theta_i}{\sqrt{\frac{E}{m_1}}\cos\theta_i + \sqrt{\frac{E-W_n^{\uparrow(\downarrow)}}{m_2}}\cos\theta_t} \,,$$

$$r^{\uparrow(\downarrow)} = \frac{\sqrt{\frac{E}{m_1}}\cos\theta_i - \sqrt{\frac{E-W_n^{\uparrow(\downarrow)}}{m_2}}\cos\theta_t}{\sqrt{\frac{E}{m_1}}\cos\theta_i + \sqrt{\frac{E-W_n^{\uparrow(\downarrow)}}{m_2}}\cos\theta_t} \,, \tag{65}$$

where $E = \frac{\hbar^2}{2m}(k_x^2 + k_y^2 + k_z^2)$, $(m_1 = m_2 = m)$.

We note that $T^{\uparrow(\downarrow)} + R^{\uparrow(\downarrow)} = 1$ is valid. In the real interface layer we have to consider the interface roughness. This can be done by using the method described in [33].

4 Conclusion

Considering the interaction energy between d and s electrons in the $3d$ transition metals the relation for the average interaction energy W_n at the given temperature and magnetic field was derived. It was shown that the energy W_n is angular and spin-dependent. For the perfect interface layer the transition cofficients $T^{\uparrow(\downarrow)}$ and the reflection one $R^{\uparrow(\downarrow)}$ were calculated. These coefficients are angular and spin dependent.

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