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SPIN FLIP ENHANCEMENT AT RESONANT TRANSMISSION

by

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ABSTRACT

The spin flip cross section for an electron which interacts by exchange in going through a layer of magnetic impurities, can be greatly enhanced in a situation of resonant transmission. We describe this effect by a one dimensional model which contains the essential physics and can be exactly solved. Besides its eventual application in problems related to the emission and reflection of spin polarized electrons, this model provides a nice and instructive quantum mechanical example.

Key-words: Spin polarization; Exchange scattering; Resonant trasmission.

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INTRODUCTION

In the course of pondering on the effect of resonances on the spin flip of photoemitted electrons induced by the exchange interaction with magnetic impurities[1], we considered a one dimensional model which, although very simple, contains the essential physics ant it is exactly solvable. It clearly illustrates the quantum mechanism leading to an enhancement of the exchange interaction in the presence of resonances. It may, therefore, be of some pedagogical value and in this sense we thought it deserved to be discussed. These ideas may also be relevant in connection to cases of strong spin relaxation of polarized electrons transmitted through magnetic layers[1,2].

MODEL

We consider an electron with energy E and spin up coming in the direction of the x-axis. The spin quantization axis is taken along the z-direction (Fig. 1). The electron interacts at the origin with an impurity spin through an exchange potential which may induce a mutual spin flip. Furthermore, two δ-like potentials, at x = a and -a, are introduced in order to provide for resonances in the transmission. The effect of the potentials is such that the electron may be reflected back into region I $(x < -a)$ or transmitted to region IV $(x > a)$ with spin up or down.

The model Hamiltonian is:

$$H = \frac{p^2}{2m^*} + G\left[\delta(x-a) + \delta(x+a)\right] - J\delta(x)\vec{s}.\vec{S} \quad , \tag{1}$$

where the first term is the kinetic energy of an electron with effective mass m*. G is the strength of the δ-like potentials at a and $-$a. The third term describes the local exchange interaction of strength J between the electron with spin $\vec{s}$ and a magnetic impurity with spin $\vec{S}$.

SOLUTION OF SCHRÖDINGER'S EQUATION

The wave function of the system can be written in spinorial form:

$$\psi_M^{I}(x) = \begin{pmatrix} [e^{ikx} + r_\uparrow e^{-ikx}]\,\phi_m \\ r_\downarrow e^{-ikx}\phi_{m+1} \end{pmatrix} \quad \text{for} \quad x \le -a$$

$$\psi_M^{R}(x) = \begin{pmatrix} [A_\uparrow^R e^{ikx} + B_\uparrow^R e^{-ikx}]\,\phi_m \\ [A_\downarrow^R e^{ikx} + B_\downarrow^R e^{-ikx}]\,\phi_{m+1} \end{pmatrix} \quad \begin{matrix} \text{with } R = II \text{ for } -a \le x \le 0 \\ \text{and } R = III \text{ for } 0 \le x \le a \end{matrix} \tag{2}$$

$$\psi_M^{IV}(x) = \begin{pmatrix} t_\uparrow e^{ikx}\phi_m \\ t_\downarrow e^{ikx}\phi_{m+1} \end{pmatrix} \quad \text{for} \quad x \ge a$$

$r_{\uparrow,\downarrow}$ and $t_{\uparrow,\downarrow}$ are the corresponding probability amplitudes for reflection and transmission with spin up and down. ϕ_m are the eigenfunction of S^Z:

$$S^Z\phi_m = m\phi_m , \tag{3}$$

and

$$k = \sqrt{2m^*E/\hbar^2} \quad , \quad \text{with} \quad E > 0.$$

$\psi_M(x)$ is a correlated function of the electron an impurity spins which takes into account that the exchange interaction conserves to z-component of the total spin $\vec{\mathcal{J}} = \vec{s} + \vec{S}$:

$$\mathcal{J}^z \psi_M(x) = M \psi_M(x) \quad , \tag{4}$$

where $M = m + \frac{1}{2}$.

The problem is now well defined, namely: the function $\psi_M(x)$ contains the asymptotic boundary conditions imposed on the electron (no electron with spin down coming from the left and no electron coming from the right), and it describes a state with fixed M which is conserved.

The continuity of the spinor wave function at $x = -a, 0,$ and a requires that:

$$\begin{aligned} L_{\uparrow,\downarrow} + r_{\uparrow,\downarrow} e^{ika} &= A^{II}_{\uparrow,\downarrow} e^{-ika} + B^{II}_{\uparrow,\downarrow} e^{ika} \\ A^{II}_{\uparrow,\downarrow} + B^{II}_{\uparrow,\downarrow} &= A^{III}_{\uparrow,\downarrow} + B^{III}_{\uparrow,\downarrow} \quad , \\ A^{III}_{\uparrow,\downarrow} e^{ika} + B^{III}_{\uparrow,\downarrow} e^{-ika} &= t_{\uparrow,\downarrow} e^{ika} \end{aligned} \tag{5}$$

where $L_{\uparrow} = e^{-ika}$ and $L_{\downarrow} = 0$.

The solution of Schrödinger's equation at the same singular points requires that[3]:

$$ik\left[A^{II}_{\uparrow,\downarrow}e^{-ika} - B^{II}_{\uparrow,\downarrow}e^{ika} - (L_{\uparrow,\downarrow} - r_{\uparrow,\downarrow}e^{ika})\right] = \frac{2m^*G}{\hbar^2}(L_{\uparrow,\downarrow} + r_{\uparrow,\downarrow}e^{ika})$$

$$ik\left[(A^{III}_{\uparrow,\downarrow} - B^{III}_{\uparrow,\downarrow}) - (A^{II}_{\uparrow,\downarrow} - B^{II}_{\uparrow,\downarrow})\right] = \frac{m^*J}{\hbar^2}\left[N_{\uparrow,\downarrow}(A^{III}_{\uparrow,\downarrow} + B^{III}_{\uparrow,\downarrow}) + F(A^{III}_{\downarrow,\uparrow} + B^{III}_{\downarrow,\uparrow})\right] \tag{6}$$

$$ik\left[t_{\uparrow,\downarrow}e^{ika} - (A^{III}_{\uparrow,\downarrow}e^{ika} - B^{III}_{\uparrow,\downarrow}e^{-ika})\right] = \frac{2m^*G}{\hbar^2}t_{\uparrow,\downarrow}e^{ika}$$

where $F = \left[(S-m)(S+m+1)\right]^{1/2}$, $N_\uparrow = m$ and $N_\downarrow = -(m+1)$.

The admixture of spin components in the 2^{nd} of eqs. (6) follows from the application of the operator $\vec{s}.\vec{S} = \left[s^z S^z + (1/2)(s^- S^+ + s^+ S^-)\right]$ to the spinor wave function. Here $s^\pm = s_x \pm is_y$ and $S^\pm = S_x \pm iS_y$, are the raising and lowering spin operators:

$$s^- S^+ \binom{1}{0}\phi_m = F\binom{0}{1}\phi_{m+1} \tag{7}$$

After some algebra one gets:

$$t_\uparrow = r_\uparrow + \frac{W^*}{W} = \frac{1 + i\left[\chi - (m+1)j'\right]}{\Delta}$$

$$t_\downarrow = r_\downarrow = \frac{-ij'F}{\Delta} , \tag{8}$$

where $j' = |W|^2 j/(2\kappa)$ and $\Delta = (1+i\chi)\left[1 + i(\chi - j')\right] + S(S+1)j'^2$

with

$$W = 1 + g\sin 2\kappa\alpha + i2g\sin^2\kappa\alpha , \tag{9}$$

and

$$\chi = 2g(g\sin 2\kappa\alpha + \cos 2\kappa\alpha) . \tag{10}$$

For convenience the following dimensionless quantities were defined: $\kappa = ka_B = \sqrt{E/\varepsilon}$, $g = G/(2ka_B\varepsilon)$, $j = J/2a_B\varepsilon$ and $\alpha = a/a_B$. Here a_B is Bohr radius and $\varepsilon = \hbar^2/2m^*a_B^2$.

$\varepsilon = 1\,Ry$ if m^* is equal to the free electron mass.

The transmission probabilities for each spin direction are given by:

$$|t_\uparrow|^2 = \frac{1 + [\chi - (m+1)j']^2}{|\Delta|^2}$$

$$|t_\downarrow|^2 = \frac{F^2 j'^2}{|\Delta|^2} \; , \tag{11}$$

and $|r_\uparrow|^2$ can be easily obtained from the condition of conservation of current probability: $1 = |r_\uparrow|^2 + |r_\downarrow|^2 + |t_\uparrow|^2 + |t_\downarrow|^2$.

For later discussion it is convenient to explicitate the density of probability of finding an electron at the origin, $|\psi_M(0)|^2$, where the exchange interaction takes place; from Eqs. (5),(6) and (2),

$$|\psi_M(0)|^2 = |W|^2(|t_\uparrow|^2 + |t_\downarrow|^2) \; . \tag{12}$$

The spin polarization, P, of the transmitted beam is defined by:

$$P = \frac{1 - T}{1 + T} \; , \tag{13}$$

where

$$T = \left|\frac{t_\downarrow}{t_\uparrow}\right|^2 = \frac{j'^2 F^2}{1 + [\chi - (m+1)j']^2} \; . \tag{14}$$

LIMIT OF SMALL EXCHANGE COUPLING

The above results can be easily interpreted in the limit of small $j'(j' << 1)$, where the effect of the δ-exchange potential on the resonance condition is negligible. In this limit we can approximate:

$$|t_\uparrow|^2 = \frac{1}{1+\chi^2} \quad , \tag{15}$$

and up to order j'^2:

$$|t_\downarrow|^2 = \frac{j'^2F^2}{1+\chi^2} \tag{16}$$

which yields

$$T = j'^2F^2 \quad . \tag{17}$$

For $G=0$, we have $|W|^2 = 1$ and our results reduce to the case of simple exchange scattering, namely: $T=(jF/2k)^2$. [2] Thus, the effect of the δ-like potentials at a and $-a$ is equivalent to that of using an effective exchange coupling parameter:

$$j_{eff} = j|W|^2 \quad . \tag{18}$$

The condition for resonant energies are obtained from the roots of χ given by eq. (10):

$$\cot 2\kappa\alpha = \mp g \tag{19}$$

The roots of χ can be uniquely labeled by an integer n such that:

$$n\pi \leq 2\kappa\alpha \leq (n+1)\pi \tag{20}$$

At resonance and for $j' << 1$, $|t_\downarrow|^2 << 1$ and $|t_\uparrow|^2 \lesssim 1$. Thus, according to eq. (12)

$$|\psi_M(0)|^2 \approx |W|^2 = (\sqrt{1+g^2} \pm g)^2 \quad . \tag{21}$$

The sign +(-) in Eq. (21) is associated to n even (odd) and the value of the corresponding wave function at the origin results from constructive (destructive) interference. Thus for even n the effect of the exchange is enhanced, while for odd n it is supressed.

NUMERICAL RESULTS AND DISCUSSION

In order to illustrate the effects mentioned above we calculated the quantities given by eqs. (11-13) in the energy range from 1 eV to 5 eV using the parameters: $a = 10\mathring{A}$, $G = 10$ eV $\mathring{A}$, $J = 0.5$ eV $\mathring{A}$, $S = 1/2$ and $m = -0.5$. While the value of J may be typical for exchange coupling between conduction electrons and a paramagnetic impurity, the other parameters, as well as the energy range, were chosen as to obtain a clear picture of the enhancement effect. In general the quantities of interest, for instance P, must be calculated for each of the $2S+1$ possible values of M, and an appropriate thermodynamical average must be taken. Here, for the sake of simplicity, the value of m was chosen to correspond to a magnetic impurity fully polarized in the -z-direction ($M = 0$).

Fig. 2a shows $|t_\uparrow|^2$ and $|t_\downarrow|^2$ as a function of the energy of the incident electron. We observe four resonances corresponding to the transmission of spin up electrons ($n = 3$ to 6), while there are only two distinguishable peaks for spin down electrons ($n=4$ and 6). For those energies the considerations made for the limit $j' \ll 1$ already hold in good degree. At lower energies, however, the transmission spectrum displays more structure due to additional interferences from the exchange potential. In Fig. 2b the corresponding spin polarization, P, of the transmitted electron and the density of probability $|\psi_M(0)|^2$ are plotted. For comparation, in the same figure, it is exhibited the spin polarization corresponding to an exchange coupling constant $J = 8$ eV Å in the absence of resonances ($G = 0$). One observes that at the particular resonant energy $E = 2.175$ eV, the condition for resonant transmission has produced an effective sixteen-fold enhancement of the exchange interaction. For $G = 0$ and $J = 0.5$ eV Å the depolarization is negligible. In fact for energies above 1 eV, $P > 0.992$.

The polarization of the reflected beam $(|r_\uparrow|^2-|r_\downarrow|^2)/(|r_\uparrow|^2+|r_\downarrow|^2)$, not displayed here, presents sharp peaks, even changing sign at the resonance energies.

We have thus shown by means of a simple model, that resonant transmission may greatly influence the exchange scattering, leading to a strong enhancement of the probability for spin flip. The situation described by this model might be realized when incident polarized electrons interact by exchange with magnetic atoms which have virtual states in the continuum[1,4].

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FIGURE CAPTIONS

Figure 1: An electron, with spin up and energy E, coming from the left interacts at the origin with an impurity spin through a local exchange potential, and with two δ-like potentials at $x = a$ and $-a$. which provide conditions for resonant transmission. The electron can be reflected back to region I, or transmitted to region IV, with spin up or down.

Figure 2a - Transmittance versus energy.

—— $|t_\uparrow|^2$, ---- $-5\times|t_\downarrow|^2$.

The numbers to the right of the peaks label the resonances (see eq. (20)).

Figure 2b - Spin polarization P and density of probability of finding the electron at the origin, $|\psi_M(0)|^2$, versus energy.

——P, and ---.05 x $|\psi_M(0)|$ for $G = 10$ eV Å and $J = 0.5$ eV Å.

——.——P, for $G = 0$ and $J = 8$ eV Å.

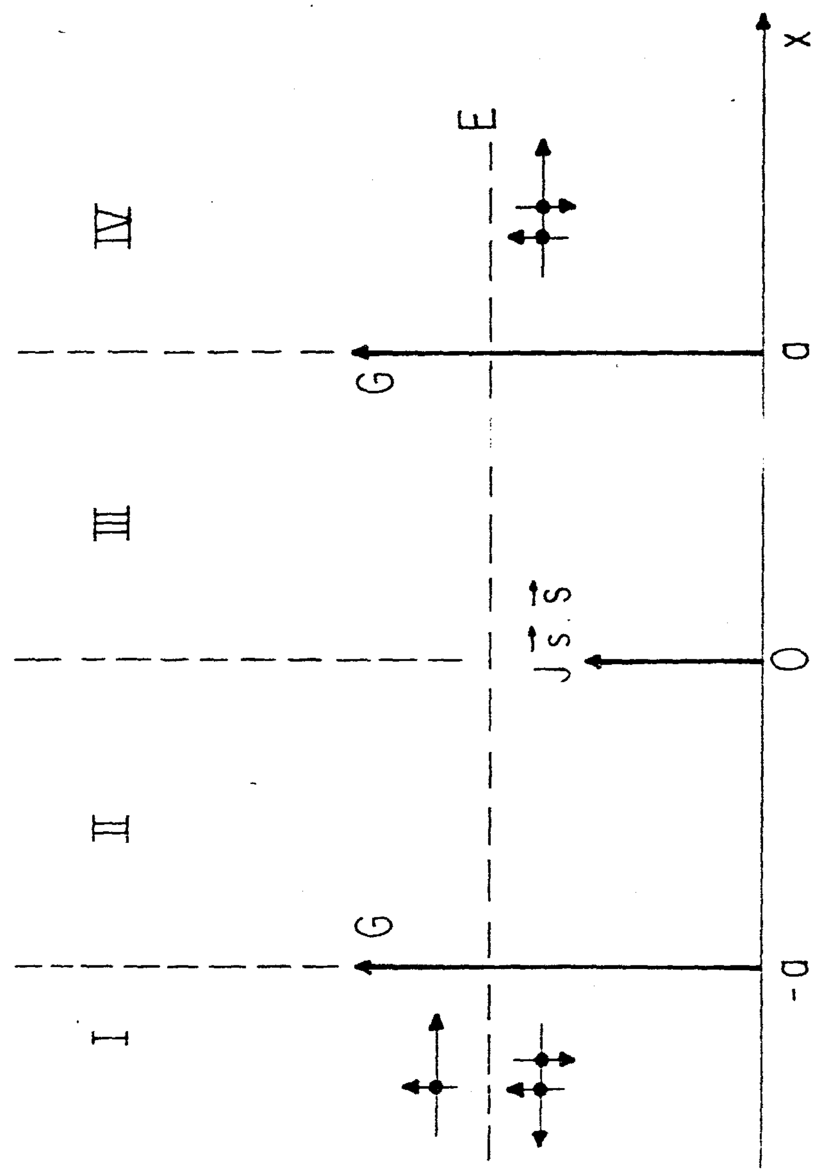

Fig. 1

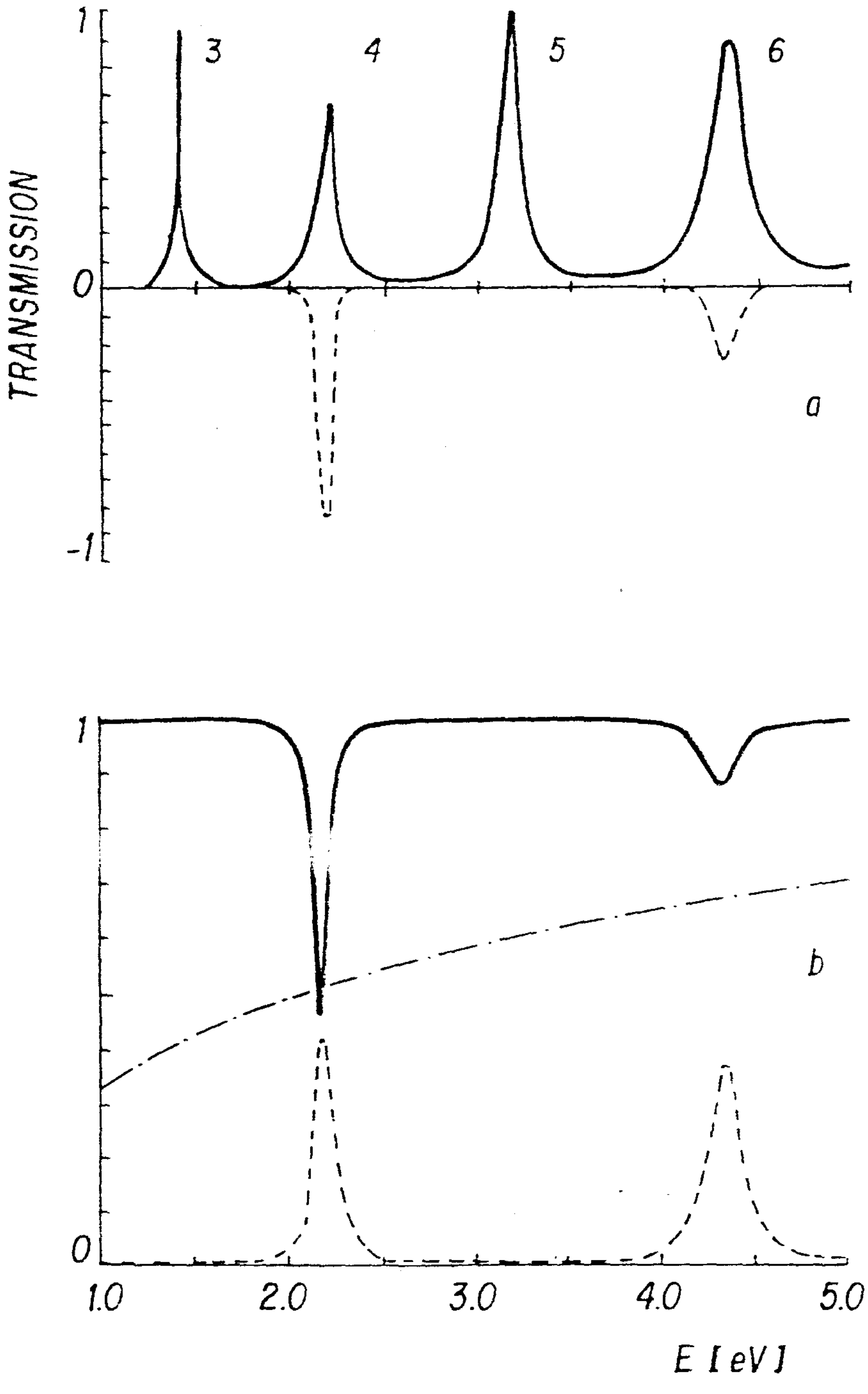

Fig. 2

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