Photovoltaic effect in a ferromagnet with spin-orbit coupling

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The effect of the appearance of an electric current induced by the electromagnetic radiation at the interface of a ferromagnet and a non-magnetic material is calculated theoretically, taking into account the Rashba spin-orbit coupling. It is shown that the electric dipole transitions between the spin subbands of the conduction electrons of a ferromagnet due to the Rashba interaction lead to a photocurrent. This current has a resonance at a frequency corresponding to the energy of the exchange splitting of spin subbands. The resonance width is determined by the spin-orbit interaction constant. The estimates show the possibility of experimental observation of this effect in specially prepared multilayer systems.

Keywords: Ferromagnet, exchange coupling, Rashba spin-orbit coupling, photovoltaic effect.

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1. Introduction

The coupling of spin and orbital degrees of freedom in ferromagnets leads to a number of unusual and interesting phenomena in optics and transport. In non-collinear ferromagnets, such phenomena as non-reciprocal light scattering [1.2] and signal generation at double frequency [3], electromagnetic wave absorption and radiation due to conductivity electrons transitions between spin subbands occur [4-8]. In non-coplanar magnetic systems there is a topological Hall effect [9-11], a rectification effect for neutrons [12–14] and electrons [15–17]. At the junction of the optical and transport phenomena there is a photovoltaic effect [18], close to the straightening effect of the alternating electric field in the non-coplanar ferromagnet [15]. This effect, like the absorption of electromagnetic radiation, is due to the conductivity electron transitions between the spin subbands of the ferromagnet under the action of the electromagnetic electric field. The non-complanarity of the magnetic moment makes it possible to couple the spin state with the movement along the allocated axis and results in the optical transitions being accompanied by the flow of electric current. This is possible due to spatially non-uniform magnetization. In the present work, a similar photovoltaic effect is calculated in a homogeneous ferromagnet in which electrodipole transitions are allowed by the Rashba spinorbital interaction.

Optical effects were previously studied in with spin-orbit interaction semiconductors placed in an external magnetic field [19]. The system considered in these works differs significantly from the ferromagnetic system considered in this paper, however, the physical essence of phenomena is close. The influence of spin-orbit interaction on electron transport in various, including ferromagnetic, systems was also investigated. The presence of persistent spin [20] and electric [21] currents in mesoscopic rings with spin-orbit interaction, as well as in the ring with the Rashba interaction, which was theoretically predicted is connected to the ferromagnet [22]. Work [23] considers photodetectors based on the two-dimensional MoS₂, which is a semiconductor and has an internal spin-orbit interaction. In work [24] in numerical calculations based on the method of nonequilibrium Green functions the effect of photoinduced voltage arising in zigzag-shaped nanoribbons from twodimensional MoS₂ having spontaneous magnetic moment was considered.

The photovoltaic effect caused by conductivity electron transitions between spin subbands under the action of the electric wave field at the boundary of the ferromagnet and heavy metal is considered in the present paper. Such systems have recently been extensively investigated due to the presence of the Dzyaloshinsky-Moriya interaction [25-28], which may, inter alia, appear because of the spin-orbital Rashba interaction [29,30]. The effect considered in the present work has a resonance at the rate of exchange splitting of the spin subbands and is therefore strong It could be used to study the properties of enough. ferromagnets and their boundaries with other substances. In particular, by observing the effect, it is possible to determine the exchange constant between the conductivity electrons and the localized electrons responsible for magnetization, to estimate the relaxation time of the electron momentum and to determine the value of the spinorbital interaction at the boundary of the ferromagnet with heavy metal.

2. Theoretical model

In order to solve the problem of rectifying electromagnetic radiation at the boundary between the ferromagnet and the non-magnetic material, the following model has been considered. The electrons of ferromagnet responsible for conductivity rectification are considered free. Their exchange interaction with the electrons responsible for the magnetization are described in the framework of the Vonsovskii *s*-*d* model. Spin-orbital interaction is considered in the form of the Rashba interaction. Thus, the Hamiltonian of conductivity electrons has the form

$$\hat{H} = \frac{\hbar^2 \hat{\mathbf{p}}^2}{2m_e} + J(\hat{\boldsymbol{\sigma}} \cdot \hat{\mathbf{M}}) - \left(\frac{\boldsymbol{\alpha}_R}{\hbar} \cdot [\hat{\mathbf{p}} \times \hat{\boldsymbol{\sigma}}]\right), \quad (1)$$

where $\hat{\mathbf{p}} = -i\hbar\nabla$ — momentum operator, $\hat{\boldsymbol{\sigma}}$ — vector of the Pauli matrices, M - magnetization vector (normalized per unit), J — exchange constant, α_R — Rashba vector. In the framework of current study, we suppose that the magnetization vector in a ferromagnet is parallel to the Cartesian axis z: $\mathbf{M} = \mathbf{e}_z$ (see Fig. 1). The most interesting case that we consider below is realized when the Rashba vector is directed perpendicular to the magnetization vector. This is due to the fact that the Hamiltonian of the Rashba spin-orbit interaction (see (1)) gives a non-zero energy contribution for the mean spin polarization directed perpendicularly to the α_R vector. One can choose the Cartesian coordinate system in such a way that $\alpha_R || \mathbf{e}_x$, as shown in Fig. 1. In the absence of the Rashba interaction, the conductivity electron energy spectrum consists of two spin subbands split into 2J:

$$\varepsilon_{\pm}^{(0)} = \frac{\hbar^2 \mathbf{k}^2}{2m_e} \pm J, \qquad (2)$$

$$\psi_{+}^{(0)} = \begin{pmatrix} 1\\ 0 \end{pmatrix} \exp(i\mathbf{k}\mathbf{r}), \quad \psi_{-}^{(0)} = \begin{pmatrix} 0\\ 1 \end{pmatrix} \exp(i\mathbf{k}\mathbf{r}) \qquad (3)$$

up to the normalization factor [31]. Here \mathbf{k} — the electron wave vector, \mathbf{r} — radius-vector, m_e — electron mass. Accounting for the Rashba interaction in a linear order of α_R results in a mixing of the spin states and correction of the spectrum dependent on electron quasimomentum

$$\varepsilon_{\pm} = \frac{\hbar^2 \mathbf{k}^2}{1m_e} \pm (J - \alpha_R k_y), \qquad (4)$$

$$\psi_{+} = \begin{pmatrix} 1 \\ i\alpha_{R}k_{z}/2J \end{pmatrix} \exp\left(i\mathbf{k}\mathbf{r} - i\frac{\varepsilon_{+}}{\hbar}t\right),$$

$$\psi_{-} = \begin{pmatrix} i\alpha_{R}k_{z}/2J \\ 1 \end{pmatrix} \exp\left(i\mathbf{k}\mathbf{r} - i\frac{\varepsilon_{-}}{\hbar}t\right).$$
(5)

Let us calculate the equilibrium electric current within this simple model in the absence of an electromagnetic wave. When calculating the "normal" current flowing in the system

$$\mathbf{j}_n = -i \, \frac{e\hbar}{2m_e} \big((\nabla \psi)^+ \psi - \psi^+ \nabla \psi \big), \tag{6}$$

 $\begin{bmatrix} \mathbf{E} & \mathbf{\alpha}_{R} \\ \mathbf{A} & \mathbf{j}_{photo} \end{bmatrix}$

Figure 1. Schematic representation of the examined system.

where the e — electron charge, it turns out to be different from zero and in the least order by the Rashba interaction has the form

$$\mathbf{j}_n = -\frac{e}{\hbar} \frac{4\pi}{3} k_{\rm F}^3 \left(\left(1 + \frac{1}{\varepsilon_{\rm F}} \right)^{3/2} - \left(1 - \frac{J}{\varepsilon_{\rm F}} \right)^{3/2} \right) [\boldsymbol{\alpha}_R \times \mathbf{M}],\tag{7}$$

where $k_{\rm F}$ and $\varepsilon_{\rm F}$ – Fermi energy and momentum. Its phenomenological form is $-f(\alpha_R)[\boldsymbol{\alpha}_R \times \mathbf{M}]$, where $f(\alpha_R)$ – some Rashba vector module function (not dependent on its direction). This "normal" current can be interpreted as follows. It is known that in a system of free electrons with Rashba interaction, a spin current arises, which has the form $J_{ij}^{S} = e_{ijk}\alpha_{Rk}$, where e_{ijk} — antisymmetric Levy–Civita tensor, i and j — spatial and spin coordinates respectively. When accounting for the exchange interaction, such spin current is converted to an electric current of the type $J_{ii}^{S}M_{i}$. In addition to "normal" current, the system has anomalous current associated with conductivity electrons having anomalous correction to speed. It is connected with the fact that the current operator has a correction due to the Hamiltonian of the Rashba spin-orbit interaction, which is determined by the formula

$$\mathbf{j}_{R} = -\frac{e}{\hbar} [\boldsymbol{\alpha}_{R} \times \psi^{+} \hat{\boldsymbol{\sigma}} \psi]. \tag{8}$$

This anomalous current turns out to be exactly equal to the "normal" one taken with minus sign. Therefore, the total electric current of $\mathbf{j}_{\Sigma} = \mathbf{j}_n + \mathbf{j}_R$ in equilibrium is zero, and there are no persistent currents in this system.

3. Interaction of ferromagnet with electromagnetic wave

The interaction of the medium with the electromagnetic wave is considered within the framework of the calibration of $\varphi = 0$, then the vector-potential of the wave has the form

$$\mathbf{A} = -\frac{ic}{2\omega} \left(\mathbf{E} + \text{c.c.} \right),\tag{9}$$

where ω — wave frequency, $\mathbf{E} = \mathbf{E}_0 \exp(-i\omega t)$ — wave electric field vector (as seen from this expression, we ignore the wave vector, i.e., only consider transitions between spin



subbands within the electrodipole approximation) c.c. — complex conjugate value. To obtain the operator of electrons interaction with an electromagnetic wave, it is necessary to modify the momentum (minimal coupling). Without the Rashba interaction (in a purely exchange approximation) the interaction operator has the form

$$\hat{H}_{em}^{(1)} = -\frac{e}{2m_e c} \left(\hat{\mathbf{p}} \mathbf{A} + \mathbf{A}\hat{\mathbf{p}}\right)$$
(10)

(here c — speed of light in vacuum) and such transitions are prohibited. Given the Rashba interaction, the $\hat{H}_{em}^{(1)}$ operator still does not give electron transitions between spin subbands. This is due to the fact that the wave functions of type (5), containing corrections due to Rashba interaction, have the form of

$$\psi_{+} \sim \begin{pmatrix} 1\\ib \end{pmatrix}, \quad \psi_{-} \sim \begin{pmatrix} ib\\1 \end{pmatrix}, \quad (11)$$

where *b* depends on k_z . When calculating the matrix element of transitions between spin subbands under the action of operator (10), in which the vector potential is determined (9) and does not depend on spatial coordinates, we get

$$\psi_{+}^{+}\hat{H}_{em}^{(1)}\psi_{-} \sim (1-ib)(\mathbf{Ek}) \begin{pmatrix} ib\\ 1 \end{pmatrix} = 0,$$
 (12)

where k-quasi-momentum of electron as before. Note that this statement is true not only in the linear order the Rashba interaction, but also in general. The reason for this is that the wave functions of electrons of form (5) are eigenfunctions of the momentum operator, although they contain spin proportional to k_z . The wave functions remain orthogonal, the average spin of electrons with a certain quasi-momentum rotates around the axis x (Rashba vector) at some angle relative to magnetization, depending on the quasi-momentum; at that, this angle is the same for both spin subbands and is independent of spatial coordinates. This means that with the chosen quasi-momentum one can switch to another spin coordinate system, in which the wave functions will be of form (3); the transition operator itself will depend on the quasi-momentum. Therefore, operator (10), which is actually proportional to the momentum operator and does not contain a spin operator, cannot cause electron transitions between states.

At the same time, the correction to the momentum in the Rashba Hamiltonian gives the interaction operator [8]:

$$\hat{H}_{em}^{(2)} = \frac{e}{\hbar c} \left(\boldsymbol{\alpha}_R [\mathbf{A} \times \hat{\boldsymbol{\sigma}}] \right).$$
(13)

This operator removes the ban on electron transitions between spin subbands for the case considered in the present paper when the Rashba vector α_R is perpendicular to magnetization **M** (Fig. 1).

Since the Rashba constant is usually small, one can limit the probability of transitions to the lower order of α_R . The probability of transitions is determined in the lowest order by the Rashba vector as follows

$$W_{\mathbf{k}\mathbf{k}'}^{\pm} = \frac{2\pi}{\hbar} \left(\frac{\alpha_R e E_z}{2\hbar\omega}\right)^2 \delta(\mathbf{k} - \mathbf{k}') \delta(\Delta\varepsilon - \hbar\omega)$$
(14)

and has a second order in α_R . Here $\Delta \varepsilon = 2J - 2k_y \alpha_R$ — electron energy gap between spin subbands (without the Rashba interaction it is equal to 2*J*). It is worth noting, that the contribution to the transitions is given only by the component of the electric field of the wave, directed along the axis *z* parallel magnetization.

The calculated transition to probability determines the photoinduced current in the considered system. Calculating, similarly to [18], the corrections $f^{(1)\pm}$ to the electron velocity distribution function $f^{\pm} = f^{(0)\pm} + f^{(1)\pm}$, related to electromagnetic wave effects on electrons, by formula

$$-\frac{f^{(1)\pm}}{\tau} = \int d^3k' W^{\pm}_{\mathbf{k}\mathbf{k}'}(f^{(0)\pm} - f^{(0)\mp}), \qquad (15)$$

where τ — relaxation time, we get a photocurrent in the form

$$\mathbf{j}_{\text{photo}} = \pi^2 \left(\frac{\alpha_R e E_z}{\hbar \omega}\right)^2 \frac{e m_e}{\hbar^3} \frac{1}{\hbar/\tau} \frac{\alpha_R}{|\alpha_R|} \mathbf{e}_y \\ \times \begin{cases} 2J, \quad |\theta| < 2k_{\text{F}-}|\alpha_R| \\ \left(\varepsilon_{\text{F}} + J - \frac{\theta^2}{8\alpha_R^2 m_e/\hbar^2}\right), \\ 2k_{\text{F}-}|\alpha_R| < |\theta| < 2k_{\text{F}+}|\alpha_R| \\ 0, \quad |\theta| > 2k_{\text{F}+}|\alpha_R| \end{cases}$$
(16)

where $\theta = \hbar \omega - 2J$,

$$k_{\mathrm{F}\pm} = \sqrt{rac{2m_e}{\hbar^2} \left(arepsilon_{\mathrm{F}} \pm J
ight)}$$

—, Fermi momentum for two spin subbands ($\varepsilon_{\rm F}$ — Fermi energy). Photocurrent (16) can be described by the phenomenological expression $g(\alpha_R)[\alpha_R \times \mathbf{M}](\mathbf{EM})^2$, where $g(\alpha_R)$ — function of the Rasba vector module. Such current is caused by a wave and flows in an nonequilibrium system, and therefore is not prohibited.

To plot the characteristic dependence of the photocurrent on frequency it is necessary to estimate the constant of spin-orbit interaction α_R . This can be done from the surface-induced Dzyaloshinsky–Moriya interaction constant for the ferromagnet and non-magnetic material [30]. It is known, for example, that at the boundary of Co/Pt (boundary of the ferromagnet/heavy metal, on which relatively strong — for magnetic materials — spin orbit interaction is realized) the constant of this interaction is $D \approx 0.4 \text{ erg/cm}^2$ [28]. Knowing the cobalt exchange hardness constant $A = 3 \cdot 10^{-6} \text{ erg/cm}^2$, we get an estimate of $\alpha_R \sim 10^{-10} \text{ eV} \cdot \text{cm}$. Then for realistic parameters current (14) takes the form shown in Fig. 2. Current is different from zero in a limited frequency range. For typical

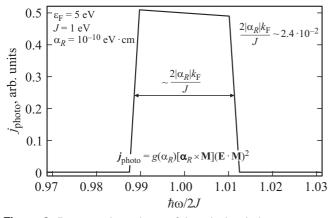


Figure 2. Resonant dependence of the calculated photocurrent on dimensionless frequency of electromagnetic wave. The parameters taken for calculation are shown in the figure.

ferromagnetic metal parameters, the center of this range corresponds to values 2*J* in the range of approximately from 0.3 to 2 eV, while the width of $2(k_{F+} + k_{F-})|\alpha_R| \approx 4|\alpha_R|k_F$ range is tens of millielectronvolts. It is possible to take into account the relaxation of the nonequilibrium spin of electrons, for example, by scattering on impurities. In this case the delta function of (14) is replaced by the Lorentz curve; this will cause the current to be different from zero for any frequency, with a pronounced resonance at a frequency of 2*J*. The resonance width will also increase.

To estimate the absolute value of current in a resonance we take the characteristic time of relaxation $\tau = 10^{-13}$ s [4]. Then for a wave field electric in the magnetization direction $E_z = 1 \text{ V/cm}$ we have an induced current of $J_{\rm photo} \sim 10^{-8} \,\text{A/cm}^2$. However, this value quadratically depends on the amplitude of the electric field (for estimations we take a small value, very far from the record), as well as on the Rashba constant. From the literature the following characteristic values of the latter for different materials are known. The greatest value of the Rashba interaction is achieved in metal heterostructures with heavy metals. When considering single surfaces, it turns out that on the surface of gold $\alpha_R = 0.33 \cdot 10^{-8} \text{ eV} \cdot \text{cm}$, and on the surface of bismuth — $0.56 \cdot 10^{-8} \text{ eV} \cdot \text{cm}$ [32]. At the interface of bismuth and silver, the constant is about an order of magnitude larger and is $\alpha_R = 3.05 \cdot 10^{-8} \text{ eV} \cdot \text{cm} [32,33].$ In the literature there is also information that in ferromagnets the Rashba interaction is suppressed and therefore the interaction constant in such a system is smaller. As mentioned above, estimating the Rashba constant for the cobalt and platinum boundaries by the Dzyaloshinsky-Moriya interaction yields $\alpha_R \sim 10^{-10} \text{ eV} \cdot \text{cm}$. This value is two orders of magnitude less than even the Rashba constant on the boundaries of nonmagnetic metals. The dimensionless value of $m_e \alpha_R / \hbar^2 k_F$, which determines the magnitude of the straightening effect considered here and is included in the second-degree response, is about $2.4 \cdot 10^{-3}$ and is very small. To enhance interband spin-orbit effects, a three-layer

system such as NiFe/Ag/Bi [33] with a very thin bismuth interlayer is possible. In this case the dimensionless value of $m_e \alpha_R / \hbar^2 k_F$ can be determined by the Bi/Ag interface and is of order 0.75. For the electric field $E_z = 1$ V/cm, this spin-orbit interaction constant yields $j_{\text{photo}} \sim 10^{-3}$ A/cm². When localizing this current on a scale of 1 Å near the boundary and the width of the sample of the order 1 cm for the field strength $E_z = 300$ V/cm have current of $I \sim 1 \mu$ A. Therefore, it is possible to experimentally observe the rectification effect at the boundary between the ferromagnet and the heavy metal with some system complexity and the use of a three-layer sample.

4. Conclusion

In this paper, the photovoltaic effect is predicted to occur at the boundary between a ferromagnet and nonmagnetic material due to the presence of the Rashba spinorbit interaction at this boundary and connected with the conductivity electron transitions between the spin subbands under the action of the electromagnetic wave electric field. This effect is resonant with a resonance at a frequency corresponding to the exchange splitting of the couductivity electron subbands of the ferromagnet, and a resonance line width determined by the product of the Rashba interaction constant α_R and the Fermi wave number k_F . In proposed three-layer system in which the ferromagnet is separated from the interface with a strong Rashba interaction by a thin layer of silver, it has been shown that it is possible to count on experimental observation of the photocurrent when it is exposed to electromagnetic radiation of sufficient intensity. The effect considered in this paper could find application in the study of the properties of ferromagnets and their boundaries with other materials. In particular, by observing the effect, it is possible to determine the exchange constant between the ferromagnet conductivity electrons and the localized electrons responsible for magnetization, to estimate the relaxation time of the electron momentum and to determine the value of the Rashba spin-orbit interaction at the boundary under study.

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Conflict of interest

The author declares that he has no conflict of interest.

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