Hole distribution in a film of a ferromagnetic semiconductor in the presence of an external electric field

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Abstract. The results of numerical calculations for the mathematical model proposed for describing the magnetization in a thin film of a ferromagnetic semiconductor at temperatures below the Curie temperature in the presence of an external electric field are presented. The theoretical prediction of the existence of a piecewise continuous solution, which describes the presence of the phase transition boundary for magnetization inside the film, is confirmed. The location of this phase transition boundary depends on the external electric field and temperature.

1. Introduction

The possibility of changing the spontaneous magnetization of a ferromagnetic semiconductor by applying an electric field was demonstrated in [1]. A thin film of a ferromagnetic semiconductor (In$_{0.03}$Mn$_{0.97}$As) 5 nm thick was placed on a substrate of different semiconductors, and the electric field, perpendicular to the film, changed its magnetization. These studies continue the earlier works [2]-[5], where a hole-like ferromagnetic order in (In,Mn)As and other materials of group III-V was studied.

In such a system, ferromagnetism is provided by the exchange interaction of holes with manganese ions by the Zener mechanism, i.e. indirect ferromagnetic interaction between ions is provided due to the ad-exchange of Vonsovsky-Ziner between holes and ions. The dependence of the density of states of the hole gas in the impurity band of energy, which noticeably overlaps with the valence band, is rather complicated. And for simplicity in the model calculation, it was assumed that this dependence is the same as in a gas of some effective mass. Theoretical assessments of these phenomena were presented in [6].

The quantum-statistical theory of influence of an electric field on the distribution of magnetization in a current-isolated ferromagnetic semiconductor was proposed in [7]. It was assumed that the manganese ions with spin 5/2 have a given spatially uniform distribution in the film, but may have a spatially non-uniform distribution of the spin direction on the axis of the easy magnetization, i.e.

$$n = n + n .$$

(1)

The distribution density of mobile holes, which had spin $\frac{1}{2}$, was not assumed to be spatially uniform $n(x) = n + n$, but the electroneutrality condition was satisfied for the system of ions and holes:

$$\int_0^L (n(x) + n(x) - n) \, dx = 0,$$

(2)

where $L$ was the thickness of the film. The magnetization density of the film was determined as

$$M(x, T) = g \left\{ \frac{5}{2} (n(x) - n) + 1 \left( n(x) - n(x) \right) \right\},$$

(3)
depending on the coordinates and the temperature. In formula (3), it was assumed that the gyromagnetic ratio \( g \) was the same for a hole and an Mn ion. The energy of the exchange interaction between Mn ions and holes was described by the formula

\[
E_{ex} = -\varepsilon_{ex} \cdot \int_0^1 \left( n_{-1/2}^{x}(x) - n_{-1/2}^{-x}(x) \right) \cdot \left( n_{1/2}^{x}(x) - n_{1/2}^{-x}(x) \right) dx, \quad \varepsilon_{ex} > 0. \tag{4}
\]

The relationships between the spatial distributions of ions and holes and the expression for the chemical potential of holes with different spin directions in the state of thermodynamic equilibrium had the forms

\[
n_{1/2}^{-x}(x) - n_{1/2}^{x}(x) = n_{-} \cdot \text{Tanh} \left( \frac{\varepsilon_{ex}}{\Theta} \cdot \left( n_{1/2}^{x}(x) - n_{-1/2}^{x}(x) \right) \right), \tag{5}
\]

\[
\mu^{x}(x) = \varepsilon_{F} - \varphi(x) \pm \varepsilon_{ex} \cdot n_{-} \cdot \text{Tanh} \left( \frac{\varepsilon_{ex}}{\Theta} \cdot \left( n_{1/2}^{x}(x) - n_{-1/2}^{x}(x) \right) \right), \tag{6}
\]

The value \( \Theta \) in (5), (6) is equal to the product \( k \cdot T \), where \( T \) is the temperature on the Kelvin scale and \( k \) is Boltzmann’s constant. The value of \( \varepsilon_{F} \) corresponds to the Fermi energy for holes of mass \( m \) in the absence of an electric field, and \( \varphi(x) \), to the potential of a self-consistent electric field in formula (6). The values of the parameters are given in atomic units in which the unit of length is \( \hbar^2 / (m_e \cdot e^2) \approx 0.529 \cdot 10^{-10} m \), and the unit of energy is \( m_e \cdot e^2 / \hbar^2 \approx 27.21 eV \).

### 2. System of 5 equations for three functions

In this paper, we propose to use asymptotic relations for polylogarithms:

\[
\text{Li}_j(-e^{-z}) \rightarrow -M^j / \Gamma(j+1), \quad \Gamma(z) = \int_0^\infty e^{-t} \cdot t^{z-1} dt,
\]

which allow us to obtain an algebraic relationship between the distribution densities of holes and their chemical potentials. Polylogarithms arise when writing Fermi-Dirac integrals. Replacing them with an asymptotic expression introduces an error in calculations that is less than one percent if the inequality \( M = \mu / \Theta > 10 \) is true. The fulfillment of this inequality should be verified for all solutions obtained in the temperature range not exceeding the Curie temperature.

This replacement allows us to write the ratio

\[
n_{1/2}^{x}(x) = 2^{-1} (\varepsilon_{ex})^{-3/2} \cdot n_{-} \cdot (\mu^{x}(x))^{3/2}, \tag{7}
\]

allowing us significantly to simplify the original task with the help of three new functions: the dimensionless potential \( \psi(x) = \varphi(x) \cdot (\varepsilon_{F})^{-1} \) of the self-consistent electric field, the density of the spatial distribution of positive hole charge \( q(x) = (n_{-})^{-1} \cdot \left( n_{1/2}^{x}(x) + n_{-1/2}^{x}(x) \right) \), and the spatial distribution of the difference \( \Delta(x) = (n_{-})^{-1} \cdot \left( n_{1/2}^{x}(x) - n_{-1/2}^{x}(x) \right) \) in the densities of holes with different spin directions.

The function \( \Delta(x) \) determines the density of magnetization by formulas (3), (5), but it itself must satisfy the equation

\[
\Delta(x) = \Lambda \left( \psi(x), \Delta(x) \right) \cdot \text{Tanh} \left( (b / T) \cdot \Delta(x) \right) / q(x),
\]

\[
\Lambda \left( \psi(x), \Delta(x) \right) = \delta \cdot \left( (3/2) \cdot (1 - \psi(x))^2 + (1/2) \cdot (\delta \cdot \text{Tanh} \left( (b / T) \cdot \Delta(x) \right))^2 \right), \tag{8}
\]

where \( q(x) \) is a function of \( \Delta(x) \) and \( \psi(x) \) according to the definition and formulas (6), (7):

\[
q(x) = (1/2) \cdot (1 - \psi(x) + a(x))^3/2 + (1/2) \cdot (1 - \psi(x) - a(x))^3/2,
\]

\[
a(x) = \delta \cdot \text{Tanh} \left( (b / T) \cdot \Delta(x) \right), \quad b = \varepsilon_{ex} \cdot n_{-} / k > 0. \tag{9}
\]
Three more equalities represent the nonlinear Poisson equation for the potential $\psi(x)$ and the boundary conditions at the lower and upper boundaries of the film:

$$\frac{d^2\psi}{dx^2} = -\gamma \cdot (q(x) - 1), \quad x \in (0, L), \quad \gamma = 4\pi \cdot n_e \cdot (\chi \cdot \varepsilon_r)^{-1} > 0,$$

$$\frac{d\psi}{dx}\bigg|_{x=0} = \frac{d\psi}{dx}\bigg|_{x=L} = -A, \quad A = E \cdot (\chi \cdot \varepsilon_r)^{-1} > 0, \quad L > 0 \quad .$$

The value $\chi$ in (10), (11) is the dielectric constant of the semiconductor.

3. Results of analysis of the system of equations (8) - (11)

At the temperature $T = 0$, the solution $\psi_0(x)$ of the boundary value problem (10) - (11) can easily be found numerically. Then from equation (9) one can easily find the charge density of holes

$$q_{0}(x) = \left(1/2\right) \cdot \left(1 - \psi_{0}(x) + \delta\right)^{3/2} + \left(1/2\right) \cdot \left(1 - \psi_{0}(x) - \delta\right)^{3/2}$$

and the magnitude of the difference $\Delta_{0}(x)$ from equation (8):

$$\Delta_{0}(x) = \delta \cdot \left\{ \left(3/2\right) \cdot \left(1 - \psi_{0}(x)\right)^{3/2} + \left(3/2\right) \cdot \left(1 + \psi_{0}(x)\right)^{3/2} \right\} / q_{0}(x) .$$

It is easy to see that the function $-\Delta_{0}(x)$ is also a solution to the problem in question. This is a manifestation of the general property of system (8) - (11): if any pair of functions $\psi(x), \Delta(x)$ is a solution, then the pair $\psi(x), -\Delta(x)$ is also a solution. Therefore, in the future we will limit ourselves to finding only positive functions $\Delta(x)$.

At very high temperatures (at temperatures above the Curie temperature) (formally for $T = \infty$) the solution $\psi_{0}(x)$ of the boundary value problem (10) - (11) can also be easily found numerically. Then from (9) it is easy to find the charge density of holes

$$q_{0}(x) = \left(1 - \psi_{0}(x)\right)^{3/2}$$

and the relation $\Delta_{0}(x) = 0$ from equation (8). Note that this solution exists at any temperature, but it corresponds to zero spontaneous magnetization.

Figures 1-5 show the results of calculations of the potential, the hole charge density and the hole density differences with opposite spin directions for the model case [7]

$$m = 2, \quad e_{g} = 5, \quad g = 2, \quad n_e = 3 \cdot 10^{21}, \quad E = 0.01$$

by formulas (8) - (14). The density of manganese ions given in (15) in atomic units corresponds to the density $2 \cdot 10^{21}$ cm$^{-3}$ in ordinary units. The thickness of the film $L = 100$ in atomic units corresponds to the thickness of 5.29 nm.

Comparison of figures 1 and 2 shows that the potential of the self-consistent electric field at temperatures above $T_c$ differs from the potential at $T = 0$ very small.
The same situation for the spatial density of holes (regardless of the spin direction) is shown by comparison of figures 3 and 4.

Figure 2. Comparison of the potentials of a self-consistent electric field with $T = 0$ and $T = \infty$ for different film thicknesses $L$.

Figure 3. Dependence of the dimensionless density (charge) of all holes, regardless of the spin direction, on the transverse film coordinate $x$ at $T = 0$ for different film thicknesses $L$.

Figure 4. Comparison of the densities (charge) of all holes, regardless of the spin direction, with $T = 0$ and $T = \infty$ for different film thicknesses $L$.

However, the value $\Delta(x)$ shows a strong change with increasing temperature from $\Delta_0(x)$ at $T = 0$ (see figure 5) to the value $\Delta_x(x) = 0$ for $x \in [0, L]$ at $T > T_c$. 
Figure 5. Dependence of the difference of the dimensionless density of holes with opposite spin orientation on the transverse film coordinate \( x \) at \( T = 0 \) for different film thickness \( L \).

The calculations by formulas (8) - (14) with \( T = 0 \) and with \( T = \infty \) are rather simple, but the calculations at temperatures from zero to the Curie temperature require an iteration procedure for each value of \( T \).

Numerical results for the function \( \Delta(x) \) at four different temperatures are shown in figure 6. When \( T = 80 \), the distributions \( \Delta(x) \) are piecewise continuous: \( \Delta(x) = 0 \) for \( x \in [0, 1.8] \) at \( T = 80 \) and \( x \in [0, 87] \) at \( T = 100 \).

![Figure 6. Distribution of the magnitude \( \Delta(x) \) at different temperatures. Distributions at \( T = 0 \) and \( T = 20 \) are hardly distinguishable.](image)

If we define the local Curie temperature \( T_c(x_0) \) in the cross section \( x_0 \) of a ferromagnetic semiconductor by the relation

\[
T_c(x_0) = \left( \frac{3}{2} \right) b \cdot \delta \cdot (1 - \psi(x_0))^{1/2},
\]

then it will exactly correspond to the data shown in figure 6.

Calculations show that \( T_c(1.8) = 80 \) and \( T_c(87) = 100 \) for the film thickness \( L = 100 \). Formula (16) is a consequence of equation (8) and allows determining the Curie temperature for the entire film thickness \( L \) as a whole by the formula

\[
T_c = T_c(L) = \left( \frac{3}{2} \right) b \cdot \delta \cdot (1 - \psi(L))^{1/2}.
\]

To ensure that the condition of applicability of the asymptotic formula for polylogarithms at temperatures \( T \leq T_c = \left( \frac{3}{2} \right) \delta \cdot b \cdot (1 - \psi(L))^{1/2} \), it is sufficient to satisfy the condition

\[
(2/3) \cdot (1 - \psi(0)) > 10 \cdot \delta^2 \cdot (1 - \psi(L))^{1/2}.
\]

For the model parameters given in (15), condition (18) is satisfied.
The density of magnetization of a film defined by formula (15) can be represented as

$$M(x, T) = g \cdot n_x \cdot m(x)$$

$$m(x) = (1/2) \left( \Delta(x) + 5 \cdot \text{Tanh} \left( \left( b / T \right) \cdot \Delta(x) \right) \right).$$

As the comparison of figures 6 and 7 shows, the difference in magnitudes is explained by the large contribution of manganese ions to the magnetization.

4. Conclusions

It is the presence of an electric field that allows one to see the appearance of the phase transition boundary for magnetization inside a film of a ferromagnetic semiconductor. The proposed theoretical formulas for connecting the local Curie temperature for the boundary with the coordinates of the boundary itself correspond to numerical calculations.

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