Inhomogeneous magnetization of a thin film of a ferromagnetic semiconductor in an electric field

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Abstract. A theoretical model describing the spontaneous magnetization of a ferromagnetic semiconductor (InMn)As film in the presence of an external electric field directed across the film is considered. It is assumed that the ions of a manganese impurity with spin 5/2 are acceptors, have a uniform spatial distribution inside the semiconductor, and do not change their position under the action of an external field. The motion of holes with spin ½ changes their spatial distribution under the action of the field. The exchange interaction between manganese ions and holes allows the formation of magnetization that is non-uniform across the film thickness.

In particular, the existence of a piecewise continuous solution describing the presence of a phase transition boundary for magnetization inside a ferromagnetic semiconductor film is shown.

1. Introduction

It is known that semiconductors and ferromagnetic materials play complementary roles in the technology of storage and the current processing of information [1]. That is why the study of phenomena occurring in a film of ferromagnetic metals on the surface of a semiconductor was the most attractive [2]-[3].

The discovery in 1992 of a hole-like ferromagnetic order in (InMn)As motivated studies on the Mn-doped GaAs semiconductor and other III-V group materials [4]-[7]. The ferromagnetic transition, which was found in GaAs at temperatures above 100 K, gave rise to the hope that a new magnetic medium would appear which could open new paths for the technology of information processing and storing [8]. Report [9] on the detection of ferromagnetism in (GaMn)N at room temperature (which was predicted in [10]) increased the interest in this class of materials.

We assume that the Mn atom acts as an acceptor upon substitution on the cation site of the III-V semiconductor, leaving the negatively charged manganese ion half-filled d shell with angular momentum L = 0 and spin S = 5/2 [8]. There are also experimental evidences [7], [11], [12] that, in these materials, the ferromagnetism occurs because of the interaction between the local moments of different Mn ions with the help of holes arising in the semiconductor valence band. To control the magnetization of the above-mentioned connections, an external electric field can be used. Detection of many new properties of semiconductor heterostructures [13]-[17] allows one to explore the physics of previously unavailable combinations of quantum structure and magnetism in semiconductors.

2. Derivation of the system of equations

In this paper, we consider a mathematical model [18] describing the magnetization of a thin (of the order of 1-10 nm) ferromagnetic semiconductor film (Ga0.95Mn0.05)As in the presence of a constant electric field perpendicular to the surface. It is assumed that the longitudinal dimensions of the film are much larger than the thickness but smaller than the size of the ferromagnetic domain.

Therefore, we here do not take into account the magnetic interactions, which are much smaller than the exchange interactions. The problem becomes one-dimensional, depending on one coordinate perpendicular to the film surface. The value of $L$ is the thickness of the film. We consider the free energy $F$ per unit surface area of the film.
\[ F = E_{ex} + F_1 + F_2 + F_3 + F_4 \]  

where \( E_{ex} \) is the energy of exchange interaction of mobile holes and fixed ions of manganese, \( F_1 \) is the free energy associated with the entropy of the distribution of spins and over the ions of manganese, \( F_2 \) is the free energy of holes, \( F_3 \) is the energy of the electrostatic field, and \( F_4 \) is the energy of interaction of mobile holes with an electrostatic field.

We introduce the density of manganese ions with the direction of spins \( \frac{5}{2} \) and \( -\frac{5}{2} \) along the easy magnetization axis \( n_{\frac{5}{2}}(x) \), \( n_{\frac{-5}{2}}(x) \) and the density of holes with different projections on this axis \( n_{\frac{1}{2}}(x), n_{\frac{-1}{2}}(x) \). The superscript here indicates the spin projection, and the subscript indicates the sign of the charge.

\[ E_{ex} = -e_{ex} \cdot \int_{0}^{L} \left( n_{\frac{5}{2}}(x) - n_{\frac{-5}{2}}(x) \right) \cdot \left( n_{\frac{5}{2}}(x) - n_{\frac{-5}{2}}(x) \right) \, dx, \quad e_{ex} > 0 \]  

\[ F_1 = -\Theta \cdot \int_{0}^{L} \left( n_{\frac{5}{2}}(x) \cdot \ln \left( \frac{n_{\frac{5}{2}}}{n_{\frac{-5}{2}}} \right) + n_{\frac{-5}{2}}(x) \cdot \ln \left( \frac{n_{\frac{-5}{2}}}{n_{\frac{5}{2}}} \right) \right) \, dx, \]  

\[ n_+ = n_{\frac{5}{2}}(x) + n_{\frac{-5}{2}}(x) \]

The value \( \Theta \) in (3) is equal to the product \( k \cdot T \), where \( T \) is the temperature on the Kelvin scale and \( k \) is Boltzmann’s constant. The second equation in (3) corresponds to the immobility of manganese ions whose total density is given by a quantity \( n_{-} \) that does not depend on the coordinate.

\[ F_2 = \int_{0}^{L} \left( \Omega(\mu^+(x), \Theta) + \mu^+(x) \cdot n_{\frac{1}{2}}(x) \right) \, dx + \int_{0}^{L} \left( \Omega(\mu^-(x), \Theta) + \mu^-(x) \cdot n_{\frac{-1}{2}}(x) \right) \, dx \]  

The thermodynamic potential \( F_2 \) of holes of mass \( m \) determines the relationship between the chemical potential \( \mu \) and the density of holes \( n_+ \). The first integral in (4) corresponds to holes, with the direction of the spin along the axis of easy magnetization, the second integral, to holes with the opposite direction of the spin. The following equations hold for the thermodynamic potential [19]:

\[ \Omega(\mu, \Theta) = \left( \frac{m \cdot \Theta}{2 \pi} \right)^{\frac{3}{2}} \cdot \Theta \cdot Li_{\frac{5}{2}} \left( -\exp(\mu / \Theta) \right), \quad Li_j(z) = \sum_{k=1}^{\infty} \frac{z^k}{k^j}, \]

\[ n_{\frac{1}{2}}(x) = -\frac{\partial}{\partial \mu} \Omega(\mu, \Theta) \bigg|_{\mu=m} = -\left( \frac{m \cdot \Theta}{2 \pi} \right)^{\frac{3}{2}} \cdot Li_{\frac{5}{2}} \left( -\exp(\mu^+(x) / \Theta) \right), \]

\[ n_{\frac{-1}{2}}(x) = -\frac{\partial}{\partial \mu} \Omega(\mu, \Theta) \bigg|_{\mu=m} = -\left( \frac{m \cdot \Theta}{2 \pi} \right)^{\frac{3}{2}} \cdot Li_{\frac{3}{2}} \left( -\exp(\mu^- (x) / \Theta) \right). \]  

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 \( m_e \cdot e^4 / \hbar^2 \approx 27,21 eV \).

When writing formulas (5), we use the notation \( Li_j(z) \) for a special function — polylogarithm. There is another notation \( PolyLog[j,z] \) in the Mathematica package. In the calculations related to formulas (5), an asymptotic formula for polylogarithms was used,

\[ Li_j(-e^{-M}) \rightarrow -M^j / \Gamma(j+1), \Gamma(z) = \int_{0}^{\frac{1}{e}} e^{-t} \cdot t^{j-1} \, dt, \]  

which ensured the 1% accuracy of calculations with \( M = \mu / \Theta > 10 \). Using asymptotic formula (6), we write the last two equations in (5) in the form

\[ n_{\frac{1}{2}}(x) = \frac{n}{2} \left( \frac{\mu^+(x)}{e_F} \right)^{\frac{3}{2}}, \quad e_F = \left( 3\pi^2 \cdot n \right)^{\frac{3}{2}} \cdot (2m)^{-1}. \]
For mobile holes, the electroneutrality condition is true:

$$\int_0^L \left( n_x^{1/2}(x) + n_x^{-1/2}(x) - n_0 \right) dx = 0.$$  \hfill (8)

The energy of the electrostatic field $F_3$ and the interaction energy $F_4$ of mobile holes with this field are determined by the following formulas in which $\chi$ is the dielectric constant of the semiconductor and $E$ is the strength of the external electrical field:

$$F_3 = \frac{\chi}{8\pi} \int_0^L \left( \frac{d\phi}{dx} \right)^2 dx,$$

$$\left. \frac{d\phi}{dx} \right|_{x=0} = \left. \frac{d\phi}{dx} \right|_{x=L} = -\frac{E}{\chi},$$

$$F_4 = \int_0^L \left( n_x^{1/2}(x) + n_x^{-1/2}(x) - n_0 \right) \cdot \phi(x) dx.$$ \hfill (11)

It is assumed that a thin ferromagnet film is separated from the metal electrodes by sufficiently thick layers of an insulator, so that the electric field does not cause a current.

As a result of minimizing the total free energy $F$ with respect to unknown functions $\phi(x), n_x^{3/2}(x), n_x^{1/2}(x), n_x^{-1/2}(x)$, we obtain four equations that allow us to find the density of the magnetic moment as a function of the coordinate $x$ and the temperature $T$:

$$M(x, T) = g \cdot \left( \frac{5}{2} \left( n_x^{3/2}(x) - n_x^{-3/2}(x) \right) + \frac{1}{2} \left( n_x^{1/2}(x) - n_x^{-1/2}(x) \right) \right).$$ \hfill (12)

In formula (12), it is assumed that the gyromagnetic ratio $g$ is the same for a hole and an Mn ion.

A variation in the free energy (1) with respect to the potential together with the boundary conditions (10) leads to the obvious boundary-value problem:

$$\frac{d^2 \phi}{dx^2} = -\frac{4\pi}{\chi} \left( n_x^{1/2}(x) + n_x^{-1/2}(x) - n_0 \right).$$ \hfill (13)

A variation in the free energy (1) with respect to the density $n_x^{3/2}(x)$ gives a local connection between the differences in manganese densities with different projections of spins on the axis of easy magnetization with the same difference in the hole densities:

$$n_x^{3/2}(x) - n_x^{-3/2}(x) = n_x \cdot \text{Tanh} \left( \frac{E_x}{\Theta} \left( n_x^{1/2}(x) - n_x^{-1/2}(x) \right) \right).$$ \hfill (14)

A variation in the free energy (1) with respect to the densities $n_x^{1/2}(x), n_x^{-1/2}(x)$ , with the electroneutrality condition (8) taken into account, leads to a local connection between the chemical potentials, the electric potential, and the difference in the hole densities with different spin directions:

$$\mu^x(x) = \varepsilon_F - \phi(x) \pm \varepsilon_\psi \cdot n_x \cdot \text{Tanh} \left( \frac{E_x}{\Theta} \left( n_x^{1/2}(x) - n_x^{-1/2}(x) \right) \right) =$$

$$= \varepsilon_F \cdot \left( 1 - \psi(x) \pm \delta \cdot \text{Tanh} \left( \frac{E_x}{\Theta} \left( n_x^{1/2}(x) - n_x^{-1/2}(x) \right) \right) \right),$$ \hfill (15)

$$\psi(x) = \phi(x) \cdot (\varepsilon_F)^{-1}, \quad \delta = \varepsilon_\psi \cdot n_x \cdot (\varepsilon_F)^{-1}.$$
3. System of 5 equations for three functions

Finally, we can write a system of five equalities for three functions: dimensionless potential \( \psi(x) \) of the self-consistent electric field, density of the spatial distribution of positive hole charge \( q(x) \) and the spatial distribution of the difference \( \Delta(x) \) in the densities of holes with different spin directions.

The transition from unknown hole densities \( n^{1/2}_1(x), n^{-1/2}_2(x) \) to the functions \( q(x) \) and \( \Delta(x) \) is determined by two equalities

\[
\begin{align*}
n^{1/2}_1(x) + n^{-1/2}_2(x) &= q(x) \cdot n, \\
n^{1/2}_1(x) - n^{-1/2}_2(x) &= \Delta(x) \cdot n,
\end{align*}
\]

\( n^{1/2}_1(x) \geq 0, \quad n^{-1/2}_2(x) \geq 0, \quad n > 0, \quad \Delta(x) \in [-1,1], \quad x \in [0,L]. \tag{16}
\]

We note that the density of magnetization (12) that we are ultimately interested in is completely determined by the function \( \Delta(x) \). With the help of the functions \( q(x), \Delta(x) \), the above five-equation system has the following form:

\[
\begin{align*}
\frac{d^2 \psi}{dx^2} &= -\gamma \cdot (q(x) - 1), \quad x \in (0,L), \quad \gamma = 4\pi \cdot n \cdot (\chi \cdot e_F)^{-1} > 0, \tag{17} \\
\frac{dq}{dx} \bigg|_{x=0} &= \frac{dq}{dx} \bigg|_{x=L} = -A, \quad A = E \cdot (\chi \cdot e_F)^{-1} > 0, \quad L > 0, \tag{18} \\
q(x) &= \left(1/2\right) \left(1 - \psi(x) + a(x)\right)^{3/2} + \left(1/2\right) \left(1 - \psi(x) - a(x)\right)^{3/2}, \\
a(x) &= \Delta \cdot \text{Tanh}[(b/T) \cdot \Delta(x)], \quad b = e_\alpha \cdot n / k > 0, \\
\Delta(x) &= \left(1/2\right) \left(1 - \psi(x) + a(x)\right)^{3/2} - \left(1/2\right) \left(1 - \psi(x) - a(x)\right)^{3/2}. \tag{19}
\end{align*}
\]

Equations (17), (18) are simply equations (13) and (10) written by using the dimensionless potential \( \psi(x) \). Equations (19)-(20) directly follow from equations (15), (16), in which the densities \( n^{1/2}_1(x), n^{-1/2}_2(x) \) are expressed through the self-consistent potential \( \psi(x) \) and the difference in the densities \( \Delta(x) \). In this case, equation (20) can be represented in a slightly different form:

\[
\Delta(x) = \Lambda(\psi(x), \Delta(x)) \cdot \text{Tanh}[(b/T) \cdot \Delta(x)] / q(x), \tag{21}
\]

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

and precisely this form will be used to solve the joint system of equations (17) - (19) and (21) to find the functions \( \psi(x) \) and \( \Delta(x) \).

In the absence of an electric field, all the functions appearing in (17) - (21) are spatially homogeneous: \( \psi(x) = \psi_0 = \text{const}, q(x) = 1, \Delta(x) = \Delta \). The values \( \psi_0, \Delta \) depend on the temperature \( T \) and are determined by solving the system of equations:

\[
\begin{align*}
\left(1 - \psi_0 + a_0(\Delta)\right)^{3/2} + \left(1 - \psi_0 - a_0(\Delta)\right)^{3/2} &= 2, \\
a_0(\Delta) &= \delta \cdot \text{Tanh}[(b/T) \cdot \Delta], \\
\Delta &= \delta \cdot \left((3/2) \cdot (1 - \psi_0)^2 + (1/2) \cdot (a_0(\Delta))^2\right) \cdot \text{Tanh}[(b/T) \cdot \Delta]. \tag{22}
\end{align*}
\]

The system of equations (22) is a special case of system (19), (21) and always has trivial solution \( \psi_0 = 0, \Delta = 0 \). This solution corresponds to the absence of magnetization (12). Note that if system (22) has solution \( \psi_0 \neq 0, \Delta > 0 \), then it also has solution \( \psi_0 \neq 0, \Delta < 0 \).

In the region \( \delta \in (0,0.25) \) and in the temperature region \( T \in \left[0, T_c^{-}\right) \), there is a solution of equations (22) with the one percent accuracy: \( \psi_0 = 0.25 \cdot (a_0(\Delta))^2, \Delta > 0 \). Here \( T_c^{-} \) is determined by the formula

\[
T_c^{-} = (3/2) \cdot b \cdot \delta. \tag{23}
\]
Obviously, $\Delta$ tends to zero as $T$ tends to the Curie temperature $T_C$. This follows from the structure of the third equation in (22).

Checking the fulfillment of the applicability condition for the asymptotic expression for polylogarithms $\mu / \Theta > 10$ for chemical potential $\mu = \mu_0 = \varepsilon_F \cdot (1 - 0.25 \cdot \delta^2 - \delta)$ in the temperature range $T \in [0, T_C)$ shows that this condition is satisfied only for $\delta < 0.225$. If we take into account the increase in the chemical potential up to $\mu = \mu_C = \varepsilon_F$ at $T = T_C$, then the limit on the value $\delta$ can be relaxed up to $\delta < 0.258$. Since $\delta = \varepsilon_{ex} \cdot (n)_{1/3}$, the possibility to use asymptotic formulas (6) with the specified accuracy imposes upper limits on the magnitude of the exchange interaction constant $\varepsilon_{ex}$ and the manganese impurity density $n_x$.

In a spatially homogeneous case (without an external electric field), the Curie temperature is determined by relation (23) at any point of the film under consideration. However, in the presence of an electric field, some non-uniformity of spontaneous magnetization occurs in the film thickness: in each section $x_0 \in [0, L]$ of thickness, there is a local critical temperature,

$$T_{cr}(x_0) = (3/2) \cdot b \cdot \delta \cdot (1 - \psi(x_0)) \quad (24)$$

Formula (24) has the following meaning: at a temperature $T = T_{cr}(x_0)$ in the region of the film $x \in [0, x_0]$, $\Delta(x) = 0$, but $\Delta(x) > 0$ in the region $x \in (x_0, L]$. The function $T_{cr}(x_0)$ is an increasing function of the coordinate $x_0$, and $T_{cr}(L)$ is the Curie temperature throughout the film thickness. Formula (24) is a consequence of equation (21) which always has trivial solution $\Delta = 0$, but there may still exist the piecewise continuous solution described above. The non-negative solution $\Delta(x) > 0$ in the area $x \in (x_0, L]$ should have the property: $\Delta(x) \to 0$ as $x \to x_0 + 0$ at a certain temperature $T = T_{cr}(x_0)$.

In the absence of an external electric field, the problem becomes spatially homogeneous and

$$T_{cr}(L) = (3/2) \cdot b \cdot \delta \cdot (1 - \psi(L))^{1/3} = (3/2) \cdot b \cdot \delta \cdot (1 - \psi_{oi})^{1/3}. \quad (25)$$

Since $\psi_{oi} = 0.25 \cdot (\Delta_i)^2$, for $\Delta = 0$ the value $\psi_{oi}$ is zero according to the second relation in (22).

Therefore, formula (25) becomes formula (23) when the external field is turned off.

4. Conclusions
The considered model allows us to estimate the spatial magnetization distribution of a thin film of a ferromagnetic semiconductor in the presence of an external electric field.

It would be much more difficult to analyze the model without detailed numerical calculations if we did not use asymptotic formulas for polylogarithms. Precisely this permits writing equations with quite observable properties. In particular, one can obtain simple approximate formulas for the dependence of the Curie temperature on the spatial coordinate across the film.

The proposed formulas well approximate the results of numerical calculations. In addition, a simple verification criterion is proposed to control the accuracy of the approximation used for polylogarithms.

It is shown that, in the model under study, there are piecewise continuous solutions that describe the presence of the phase transition boundary for magnetization inside the film of a ferromagnetic semiconductor. The location of this phase transition boundary depends on the external electric field and the temperature.

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