Spin polarization and magnetization of conduction-band dilute-magnetic-semiconductor quantum wells with non-step-like density of states

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Abstract. We study the magnetization, $M$, and the spin polarization, $\zeta$, of n-doped non-magnetic-semiconductor (NMS) / narrow to wide dilute-magnetic-semiconductor (DMS) / n-doped NMS quantum wells, as a function of the temperature, $T$, and the in-plane magnetic field, $B$. Under such conditions the density of states (DOS) deviates from the occasionally stereotypic step-like form, both quantitatively and qualitatively. The DOS modification causes an impressive fluctuation of $M$ in cases of vigorous competition between spatial and magnetic confinement. At low $T$, the enhanced electron spin-splitting, $U_{os}$, acquires its bigger value. At higher $T$, $U_{os}$ decreases, augmenting the influence of the spin-up electrons. Increasing $B$, $U_{os}$ increases and accordingly electrons populate spin-down subbands while they abandon spin-up subbands. Furthermore, due to the DOS modification, all energetically higher subbands become gradually depopulated.

1. Introduction

During the last few years, the advancement of growth, characterization and understanding of transition-metal-doped III-V semiconductors has been impressive. In magnetic semiconductor heterostructures based e.g. on (Ga,Mn)As, Mn substitutes a small fraction of cations providing holes and local magnetic moments. Many new phenomena have been accordingly brought to light e.g. tunnel magnetoresistance, spin-dependent scattering, interlayer coupling due to carrier polarization, electrical electron and hole spin injection, and electric field control of ferromagnetism [1]. Most of the structures used are based on III-V magnetic semiconductors like (In,Mn)As and (Ga,Mn)As which utilize the valence band [1]. The highest ferromagnetic transition temperature, $T_C$, reported so far for III-V-based valence-band magnetic semiconductors is 110 K for (Ga,Mn)As and 60 K for (In,Mn)As, for bulk materials, while $T_C$ can reach 150 K for some heterostructures [1].

On the other hand, in II-VI materials, Mn provides only local magnetic moments, and the corresponding heterostructures e.g. ZnSe/Zn$_{1-x}$Cd$_x$Mn$_y$Se/ZnSe utilize the conduction band.
Carriers are usually provided by donor-doping the barriers, e.g. with Cl. Magneto-optical experiments in ZnSe/Zn$_{1-x-y}$Cd$_x$Mn$_y$Se/ZnSe quantum wells have shown that the optical transitions are in the violet to blue range ($\sim$ 410 nm to 470 nm) [2]. Furthermore, the existence of ferromagnetic order in n-doped (Cd,Mn)Te based structures -at extremely low temperatures- has been suggested both experimentally and theoretically [3, 4].

In the present article we investigate such a system where the conduction-band can be exploited for spintronic applications. Specifically, we analyze II-VI-based n-doped non-magnetic-semiconductor (NMS) / narrow to wide dilute-magnetic-semiconductor (DMS) / n-doped NMS quantum wells (QWs) like e.g. ZnSe/Zn$_{1-x-y}$Cd$_x$Mn$_y$Se/ZnSe. Moreover, we use an in-plane magnetic field as a tool, in order to achieve non-step-like density of states (DOS).

2. Theory

Under a magnetic field, applied parallel to the interfaces, the density of states deviates from the ideal step-like form both quantitatively and qualitatively [5], i.e. it becomes:

$$n(E) = \frac{A\sqrt{2m^*}}{4\pi^2\hbar} \sum_{i,\sigma} \int_{-\infty}^{+\infty} dk_x \Theta(E - E_{i,\sigma}(k_x)) \sqrt{E - E_{i,\sigma}(k_x)}.$$  \hspace{1cm} (1)

The QW is along the $z$ axis and the magnetic field $B$ is applied along the $y$ axis. $\Theta$ is the step function, $A$ is the $xy$ area of the structure, $m^*$ is the effective mass. $E_{i,\sigma}(k_x)$ are the spin-dependent $xz$-plane eigenenergies. We notice that in the general case, $E_{i,\sigma}(k_x)$ must be self-consistently calculated [7, 5, 6, 8]. Equation (1) is valid for any type of interplay between spatial and magnetic confinement i.e. for narrow as well as for wide QWs. The $k_x$ dependence in Eq. (1) increases the numerical cost by a factor of $10^2 - 10^3$ in many cases. In the limit $B \to 0$, the DOS retains the occasionally stereotypic staircase shape with the ideal step $\frac{m^* A}{\pi \hbar^2}$ for each spin. The opposite asymptotic limit of Eq. (1) is that of a simple saddle point, where the DOS diverges logarithmically. The DOS modification significantly affects the physical properties e.g. the spin-subband populations, the internal and free energy, the entropy and the magnetization. We have lately calculated [5] these properties at very low temperature. We have also predicted an impressive fluctuation of the magnetization in cases of strong competition between spatial and magnetic confinement [5].

![Figure 1](image1.png)  
**Figure 1.** Magnetization, $M$, as a function of $B$ for three characteristic well widths, $L$. For $L = 30$ nm, there is a strong competition between spatial and magnetic confinement.

![Figure 2](image2.png)  
**Figure 2.** The spin polarization tuned by varying the temperature and the magnetic field: (a) $\zeta(T)$, $T = 0$ to 300 K, $B = 1$ or 10 or 20 Tesla, and (b) $\zeta(B)$, $B = 0$ to 20 Tesla, $T = 1$ or 5 or 20 or 100 K. $L = 10$ nm.
Figure 1 depicts the magnetization, $M$, as a function of $B$ for three characteristic well widths, $L$, in a representative “low temperature” case. For $L = 10\, \text{nm}$ the spatial confinement dominates and the dispersion, $E_{i,\sigma}(k_z)$, is almost parabolic. The DOS is an “almost perfect staircase”. Increasing $B$, the “height” of its steps is slightly augmented. The $L = 10\, \text{nm}$ curve mirrors this gradual increase of the DOS by a few percent. For $L = 60\, \text{nm}$ the system is basically a spin-down bilayer one. On the contrary, for $L = 30\, \text{nm}$, there is a strong competition between spatial and magnetic confinement, resulting in a severe DOS modification, which leads to an impressive fluctuation of the magnetization. Another way to describe this transition, is that the “Fermi surface” (a sphere for very low $B$), is gradually distorted and split into two parts. The variation of the temperature, $T$, affects the spin polarization. The spin polarization is also influenced by the magnetic field, in an antagonistic manner i.e. $B$ tends to align the spins. Furthermore, for each type of spin population, the in-plane magnetic field -via the distortion of the Fermi surface- redistributes the electrons between the subbands.

In the present system, the electron spin-splitting, $U_{\text{osr}}$, is enhanced i.e. it is not proportional to the cyclotron gap, $\hbar \omega_c$, i.e. \cite{9, 10}

$$U_{\text{osr}} = \frac{g^* m^*}{2m_e} \hbar \omega_c - y N_0 J_{\text{sp-d}} S B S(\xi) = \alpha + \beta. \quad (2)$$

$g^* = 1.37$ is the g-factor and $m^* = 0.16 m_e$ is the effective mass of the conduction-band electron in ZnSe \cite{11}. $m_e$ is the electron mass. The term $\beta$ arises from the exchange interaction between the conduction electron and the Mn$^{+2}$ cations. $N_0$ is the concentration of cations. $B_S(\xi)$ is the standard Brillouin function, while \cite{10, 12} $\xi = \frac{2 \mu_B B \frac{S}{2} J_{\text{sp-d}} S^2 n_{\text{down}}^2 - n_{\text{up}}^2}{k_B T}$. $k_B$ is the Boltzmann constant. The g factor of Mn, $g_{\text{Mn}} = 2$. $\mu_B$ is the Bohr magneton. The spin of the Mn$^{+2}$ ion is $S = 5/2$. The coupling strength due to the spin-spin exchange interaction between the d electrons of the Mn$^{+2}$ ions and the s- or p-band electrons, $J_{\text{sp-d}}$, is negative for conduction band electrons. $n_{\text{down}}(r)$ and $n_{\text{up}}(r)$ are the spin-down and spin-up electron concentrations. Notice that $n_{\text{down}}(r) - n_{\text{up}}(r)$ is positive for conduction band electrons. Finally, for conduction band electrons, the spin polarization can be defined by $\zeta = \frac{N_{s,\text{down}} - N_{s,\text{up}}}{N_s}$. $N_s = N_{s,\text{down}} + N_{s,\text{up}}$ is the free carrier two-dimensional concentration.

### 3. Results and discussion

At low enough $T$, $B_{5/2}(\xi) \simeq 1$. If $-y N_0 J_{\text{sp-d}} (y = 0.035)$ is taken \cite{9} $0.13$ Hartree$^*$, then $\beta = 0.325$ Hartree$^*$. For ZnSe, $1$ Hartree$^* \approx 70.5$ meV, thus $\beta \approx 23$ meV. For ZnSe, $\alpha \approx \tau 10^{-3}$ Hartree$^*$, where $\tau$ is the arithmetic value of $B$ in Tesla. Thus the term $\alpha$ is one or two orders of magnitude smaller than the term $\beta$. If the conduction band offset is $1$ Hartree$^*$ \cite{9}, then the spin splitting is $\sim \frac{1}{3}$ of the conduction band offset. ZnSe has a sphalerite-type structure and the lattice constant is $\sim 0.567 \, \text{nm}$. Hence, $-J_{\text{sp-d}} \approx 12 \times 10^{-3}$ eV nm$^3$. This is one order of magnitude smaller than the value commonly used for the III-V Ga(Mn)As valence band system ($J_{pd} = 15 \times 10^{-2}$ eV nm$^3$) \cite{10, 12}. Due to the small value of $J_{\text{sp-d}}$ the influence of the feed-back mechanism due to the difference between spin-down and spin-up concentrations is negligible in the present system. At higher temperatures, $B_{5/2}(\xi)$ cannot be approximated with $1$. As $k_B T$ increases, $\xi$ decreases, and consequently $B_{5/2}(\xi) < 1$. In other words, increasing $T$, the spin-splitting decreases allowing enhanced contribution of the spin-up electrons to the system’s properties \cite{13}. Figure 2 depicts the spin polarization of a $L = 10\, \text{nm}$ structure, tuned by varying the temperature and the magnetic field. The case of a narrow $L = 10\, \text{nm}$ structure with almost parabolic dispersion is presented here.

Figure 3 and Fig. 4 depict the subband populations as a function of $B$, for two different well widths, namely Fig. 3 for $L = 30\, \text{nm}$ and Fig. 4 for $L = 60\, \text{nm}$. $T = 20\, \text{K}$, in both cases. We use the symbols $00$ for the ground-state spin-down-subband, $10$ for the 1st excited...
spin-down-subband, 01 for the ground-state spin-up-subband and finally 11 for the 1st excited spin-up-subband. We observe that there are two mechanisms which cause depopulations: (a) The Fermi surface distortion (or equivalently the DOS modification) which depopulates all excited states, regardless of their spin [7]. (b) The increase of spin-splitting which eliminates spin-up electrons. For the very wide quantum well (L = 60 nm), as expected, the four spin-subbands are almost equally populated for B = 0.

4. Synopsis

We have described how the spin polarization and the magnetization are influenced by the temperature and the in-plane magnetic field in conduction-band, narrow to wide, n-doped non-magnetic-semiconductor (NMS) / dilute-magnetic-semiconductor (DMS) / n-doped NMS structures. It is our opinion that these structures offer a valuable field for spintronics and enhanced attention to their properties under in-plane magnetic field is recommended.

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