Magnetic properties of parabolic quantum dots in the presence of the spin–orbit interaction

O. Voskoboynikov[a)]
National Chiao Tung University, 1001 Ta Hsueh Road, Hsinchu 300, Taiwan, Republic of China

O. Bauga
Kiev Taras Shevchenko University, 64 Volodymirska st., 01033 Kiev, Ukraine

C. P. Lee
National Chiao Tung University, 1001 Ta Hsueh Road, Hsinchu 300, Taiwan, Republic of China

O. Tretyak
Kiev Taras Shevchenko University, 64 Volodymirska st., 01033 Kiev, Ukraine

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We present a theoretical study of the effect of the spin–orbit interaction on the electron magnetization and magnetic susceptibility of small semiconductor quantum dots. Those characteristics demonstrate quite interesting behavior at low temperature. The abrupt changes of the magnetization and susceptibility at low magnetic fields are attributed to the alternative crossing between the spin–split electron levels in the energy spectrum, essentially due to the spin–orbit interaction (an analog of the general Paschen–Back effect). Detailed calculation using parameters of InAs semiconductor quantum dot demonstrates an enhancement of paramagnetism of the dots. There is an additional possibility to control the effect by external electric fields or the dot design.
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I. INTRODUCTION

With recent advanced technologies it has become possible to study in detail the electron energy levels of different kinds of quantum dots and operate with a precise number of electrons or with stabilized chemical potential in the dots.[1,2] Orbital and spin magnetization of those systems has been under an extensive study during the recent decade.[3–12] The point of interest is that the magnetization provides with information about multiparticle dynamics of the dots in an external magnetic field. In addition, recent development of spintronics requires an extensive study of magnetic properties of nanosystems.[13–16] The spin states in the quantum dots are promising candidates for realizations of qubit in the quantum computing.[17] Therefore, the study of the magnetic properties of quantum dots despite of the fascinating physics can provide us with additional tools to control the electronic magnetism in nanoscale structures.

The electron spin controls design of the energy shells and magnetic properties of semiconductor quantum dots.[1,18–20] Among other spin dependent interactions, the spin–orbit interaction (the interaction between orbital angular and spin momenta[21,22]) plays an observable role in the energy spectrum formation for III–V semiconductor nanostructures. When the potential through which the carriers move is inversion asymmetric one, the spin–orbit interaction removes the spin degeneracy of the energy levels even without external magnetic fields. It sufficiently alters the electronic properties of semiconductor nano-structures.[23–28]

The purpose of this article is to study possible consequences of the spin–orbit interaction in magnetic properties of quantum dots at weak magnetic fields. We calculate the magnetization and susceptibility of a cylindrical quantum dot with the parabolic confinement potential for electrons when the spin–orbit interaction is included into consideration. The effective single-particle lateral parabolic potential describes quite well the observed properties of quantum dots (artificial atoms) with a small number of electrons.[29,30] Application of a magnetic field along the dot axes generates a complicated structure of the electron energy levels and the theoretical analysis of the parabolic quantum dots in magnetic fields achieves a rich physics. The energy level behavior and thermodynamical properties of parabolic quantum dots in magnetic fields were discussed extensively.[4,6,11,12] Recently the well pronounced spin splitting was found for the parabolic confinement potential model of semiconductor quantum dots with parameters of InSb and InAs.[28] The spin splitting at zero magnetic field leads to a crossing of the energy levels in weak external magnetic fields (similarly to the general Paschen–Back effect) and can provide unusual magnetic properties of the quantum dots.

In order to examine evidences of the impact of the spin–orbit interaction on the magnetization and susceptibility of quantum dots we focus on the Rashba term[22,25] in the spin–orbit interaction potential. A generalization with including of the Dresselhaus interaction[21] can be done straightforward in future studies.

II. MODEL OF THE QUANTUM DOT

In the presence of a uniform magnetic field B applied along the axis of the dot (z direction) the single-particle Hamiltonian in the lateral cylindrical coordinates $\{\rho,\phi\}$ is written as[28]

[a)]Author to whom correspondence should be addressed; electronic mail: vam@cc.nctu.edu.tw

$$H = -\frac{\hbar^2}{2m(E)}\left[\frac{\partial}{\rho\partial\rho}\rho\frac{\partial}{\partial\rho} + \frac{1}{\rho^2}\frac{\partial^2}{\partial\phi^2}\right] - \frac{i}{2}\hbar\omega_c(E,B)\frac{\partial}{\partial\phi} + \tfrac{1}{8}m(E)\omega_c^2(E,B)\rho^2 + V_c(\rho) + V_{so}^R(\rho,\phi) + \tfrac{1}{2}\sigma_z\mu_B g(E)B, \tag{1}$$

where

$$V_c(\rho) = \tfrac{1}{2}m(E)\omega_0^2\rho^2, \tag{2}$$

is the effective parabolic lateral confinement potential, $\hbar\omega_0$ is the characteristic confinement energy, the electron effective mass is given by[25,31]

$$\frac{1}{m(E)} = \frac{1}{m(0)}\frac{E_g(E_g+\Delta)}{(3E_g+2\Delta)}\left[\frac{2}{E+E_g} + \frac{1}{E+E_g+\Delta}\right] \tag{3}$$

[E denotes the electron energy in the conduction band, $m(0)$ is the conduction-band-edge effective mass, E_g and Δ are the main band gap and the spin–orbit band splitting, respectively]

$$\omega_c(E,B) = \frac{eB}{m(E)}$$

is the electronic cyclotron frequency, where σ_z is the Pauli z matrix

$$g(E) = 2\left[1 - \frac{m_0}{m(E)}\frac{\Delta}{3(E_g+E)+2\Delta}\right] \tag{4}$$

is the effective Lande factor of the semiconductor,[32] $\mu_B = e\hbar/2m_0$ is the Bohr magneton, e is the electron charge, and m_0 is the free electron mass.

The Rashba spin–orbit interaction term in Eq. (1) is given by[25,27,33,34]

$$V_{\mathrm{so}}^R(\rho,\phi) = \boldsymbol{\sigma}_z\alpha\frac{dV_c(\rho)}{d\rho}\left(\mathbf{k}_\phi + \frac{e}{2\hbar}B\rho\right), \tag{5}$$

where $\mathbf{k}_\phi = -i(1/\rho)\partial/\partial\phi$, and α is the spin–orbit coupling parameter within the Rashba approach.[25]

The eigenenergies of the Hamiltonian can be obtained by means of a self-consistent solution of the following equation:[28]

$$E_{n,l,\sigma} = \hbar\Omega_\sigma(E_{n,l,\sigma},B)(2n+|l|+1) + l\frac{\hbar\omega_c(E_{n,l,\sigma},B)}{2} + s\left[\frac{\mu_B}{2}g(E_{n,l,\sigma})B + l\alpha m(E_{n,l,\sigma})\omega_0^2\right], \tag{6}$$

where

$$\Omega_\sigma^2(E,B) = \omega_0^2 + \frac{\omega_c^2(E,B)}{4} + s\alpha\frac{m(E)\omega_0^2}{\hbar}\omega_c(E,B),$$

n, l, and $s = \pm 1$ refer to the main quantum number, orbital quantum number, and the electron spin polarization along the z axis correspondingly. The electron energy levels Eq. (6) with different spins and the same angular momentum $|l| > 0$ due to the spin–orbit interaction are split at $B = 0$ and cross with increasing of the magnetic field [see inset in Fig. 1(b)].[28] Note that the levels with parallel spin and angular momentum (antiparallel spin and angular momentum) remain twofold degenerated. This is the well known Kramers degeneracy.

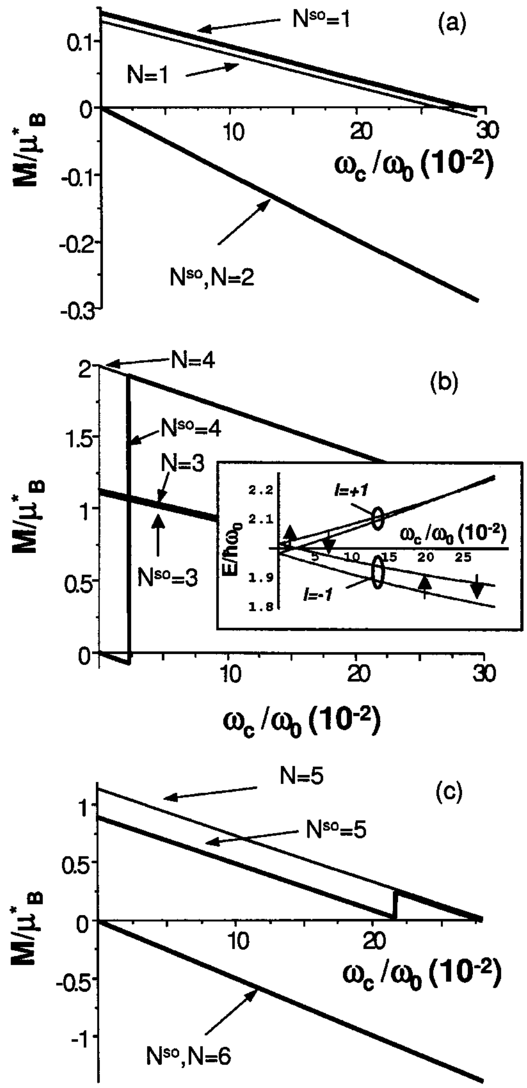

FIG. 1. Magnetization of InAs parabolic quantum dot with and without spin–orbit interaction: (a) for one and two electrons; (b) for three and four electrons (inset shows the dot energy levels for $|l|=1$ with the spin–orbit interaction included, arrows refer to the spin polarizations); (c) for five and six electrons. Index "so" marks calculations with spin-orbit interaction, $\mu_B^* = e\hbar/2m(0)$.

The first crossing point for the lowest spin-split levels ($|l|=1$) is determined by

$$\frac{\Phi}{\Phi_0} \approx \frac{\Delta E}{\hbar\omega_0} \ll 1, \tag{7}$$

where Φ is the magnetic flux in the dot area, ΔE is the energy spin splitting at $B=0$, and Φ_0 is the magnetic flux quantum. The second crossing point occurs at[28]

$$\frac{\Phi}{\Phi_0} = \frac{2\Delta E}{(2\Delta E + g\hbar\omega_0)}. \tag{8}$$

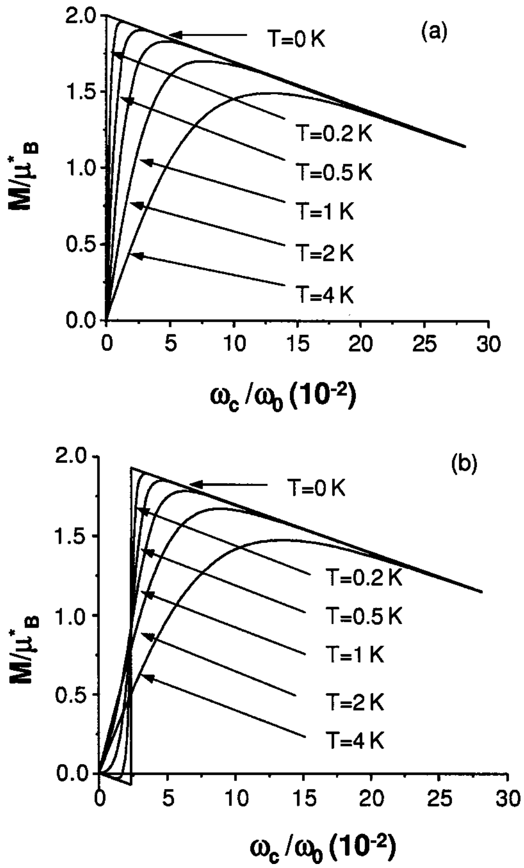

FIG. 2. Temperature dependence of InAs four electron quantum dot magnetization (a) without and (b) with spin–orbit interaction.

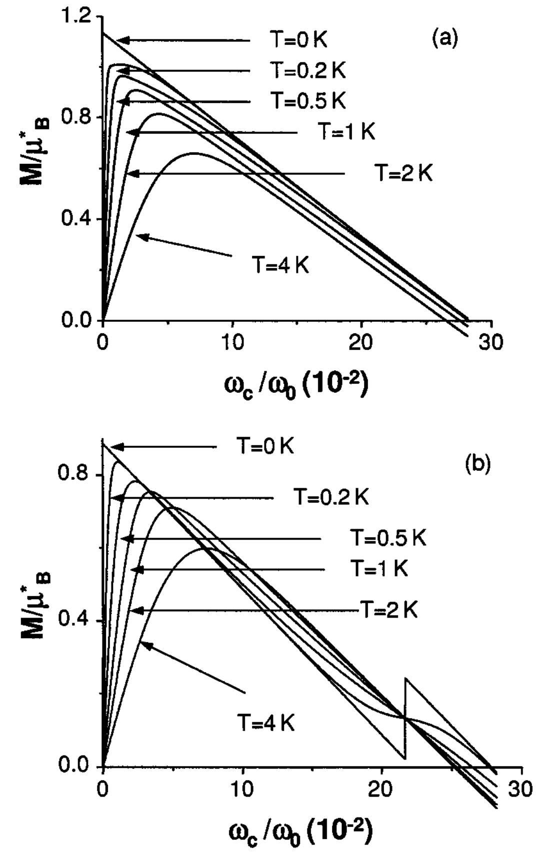

FIG. 3. Temperature dependence of InAs five electron quantum dot magnetization (a) without and (b) with spin–orbit interaction.

Being interested in the impact of the spin–orbit interaction on the magnetic properties of the dots we confine ourself on relatively weak magnetic fields as it is followed from Eqs. (7) and (8).

In our calculation we fix only the thermal average of the total electron number to a given value N. In the case of the fixed number of electrons one should use the canonical ensemble description.[6–8,35] The thermal average of the total magnetization M and magnetic susceptibility χ of the system connected to a reservoir and with a fixed chemical potential[35] are given by

$$M=\sum_{n,l,s}\left(-\frac{\partial E_{n,l,\sigma}}{\partial B}\right)f(E_{n,l,\sigma}-\xi), \tag{9}$$

and

$$\chi=\frac{\partial M}{\partial B}, \tag{10}$$

where $f(E)$ is the Fermi distribution function, and ξ is the chemical potential of the system determined by the following equation:

$$N=\sum_{n,l,s} f(E_{n,l,\sigma}-\xi). \tag{11}$$

III. CALCULATION RESULTS

The ultimate consequence of the spin–orbit interaction in the dot magnetization (the magnetic momentum of the dot) we describe first at zero temperature for quantum dots with few electrons. For small InAs quantum dots we choose $m(0)=0.04\,m_0$ (the tuned parameter from Ref. 36), $E_g=0.42$ eV, $\Delta=0.38$ eV, $\alpha=1.1$ nm^2, and $\hbar\omega_0=0.019$ eV.[28,31,37] The calculated magnetization of dots with 1–2, 3–4, and 5–6 electrons (when we consecutively fill up the energy levels of the dot to the shell with $n=0$, $|l|=1$) is shown in Fig. 1. For comparison, the magnetization for the same number of electrons but without the spin–orbit interaction is also presented in the figure. The magnetization calculated without the spin–orbit interaction demonstrates a clear shell filling behavior: for $N=2$, 6 [closed shells, see Figs. 1(a) and 1(c)] the magnetic momenta are canceled out at $B=0$; for $N=1$, 3, 4, 5 [partially occupied shells, see Figs. 1(a), 1(b), 1(c)] the magnetization takes a positive value at $B=0$. Our calculation results suggest that the spin–orbit interaction keeps the cancellation for the closed shells and slightly changes the magnetization for $N=1$, 3.[6]

The most interesting result we obtain for dots with four and five electrons. The spin–orbit splitting partially lifts up the degeneracy of $(0,\pm1,\pm1)$ levels and changes the electron structure making $E_{0,\pm1,\pm1}>E_{0,\mp1,\pm1}$.[28] This assures the magnetization to be zero at $B=0$ for dots with four electrons in contrast to the case without the spin–orbit interaction. When we increase magnetic field strength and reach condition (7) (at $B\approx0.14$ T) the crossing between levels $E_{0,1,-1}$ and $E_{0,-1,1}$ occurs [see inset in Fig. 1(b)]. For the quantum dot with four electrons the level crossing provides a sharp

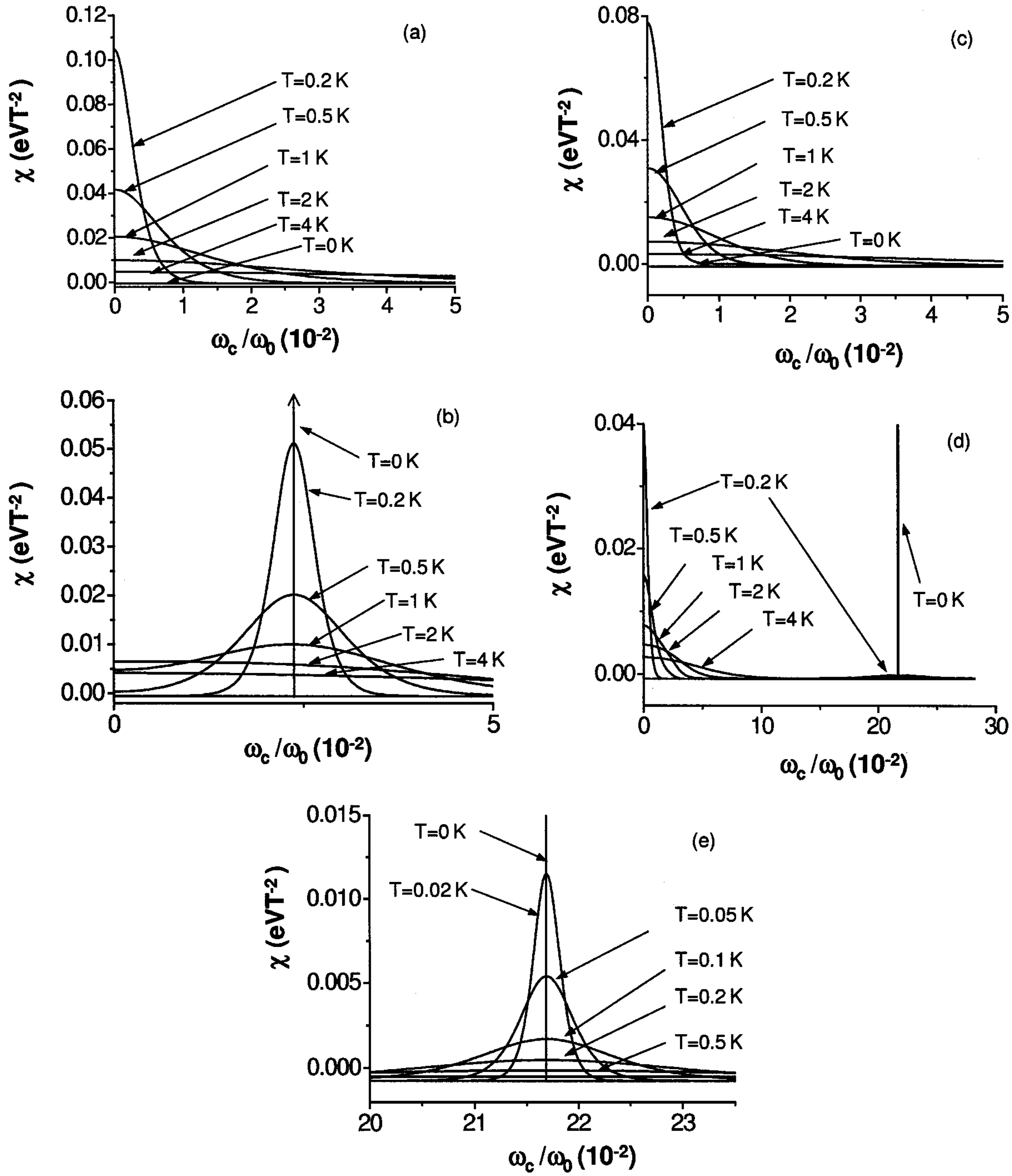

FIG. 4. Temperature dependence of the susceptibility of InAs parabolic quantum dot: (a) $N=4$; (b) $N^{so}=4$; (c) $N=5$; (d) $N^{so}=5$; and (e) $N^{so}=5$, at the region of the second peak.

jump in the magnetization. For the quantum dot with five electrons the jump reflects a crossing between $E_{0,1,-1}$ and $E_{0,1,1}$ levels for a higher magnetic field [condition (8)]: $B \approx 1.4\,\mathrm{T}$.

At a low but finite temperature $k_B T \ll \hbar\omega_0$ (k_B is the Boltzmann constant) the magnetization for dots with $N=1$, 2, 3, 6 follows the well known rule: totally occupied shells keep provide diamagnetic properties of the systems and partially filled shells demonstrate paramagnetic peaks. The peaks decrease exponentially [$\sim\exp(-k_B T/\hbar\omega_0)$] and the magnetization approaches the Landau diamagnetism limit when $k_B T \sim \hbar\omega_0$.[35]

The magnetization for the dot with four electrons at different temperatures is presented in Fig. 2. In this case $M \to 0$ for $B \to 0$ and $T \neq 0$. When the magnetic field increases the magnetization demonstrates the paramagnetic peak. The spin–orbit interaction shifts the position of the peak. For the dot with five electrons we obtain an additional paramagnetic peak at a higher magnetic field due to the crossing of the $E_{0,1,-1}$ and $E_{0,1,1}$ levels [it is shown in Fig. 3(b)].

The above described peculiarities in the magnetization of dots due to the spin–orbit interaction generate well understandable features of the magnetic susceptibility. In Fig. 4 we show χ as a function of B for dots with four and five electrons at different temperatures. At nonzero temperatures without the spin-orbit interaction we obtain the paramagnetic peak near $B=0$ [see Figs. 4(a), 4(c)]. The spin–orbit interaction shifts the peak to the field defined by Eq. (7) for dots with four electrons [see Fig. 4(b)]. In the case of the dot with five electrons we observe at low temperature two peaks: near $B=0$ (the ordinary one) and at the field defined by Eq. (8) (generated by the spin–orbit interaction) [see Figs. 4(d), 4(e)]. Clearly, the differential susceptibility demonstrates unusual behavior, which is generated by the jumps of the magnetization and certainly occur only when the spin–orbit interaction is included.

One can control the spin coupling parameters in planar semiconductor systems by means of external or built-in electric fields.[22,25] By variations of the fields one can change magnitudes of the parameters. From the above it appears that the peaks of the magnetic susceptibility which are generated by the spin–orbit interaction should have the following interesting properties. It is possible to perform a switching between the configuration presented in Fig. 4(a) and the configuration of Fig. 4(b) for dots with four electrons by means of the external electric field or the design of quantum dots. The switching is also possible between the configurations of Fig. 4(c) and the configurations of Fig. 4(d) for dots with five electrons.

IV. CONCLUSIONS

Before we conclude, we would like to mention that in this article the Coulomb interaction between electrons is neglected for simplicity. The crossing in the energy levels can be generated also by including the electron–electron interaction into consideration. But in this case the crossing occurs between levels with different l and in stronger magnetic fields.[3–5,38,39] To fully understand the described effects a many electron problem should be solved.[2,30] However, the recent investigation[36] suggests that the effect of the electron–electron interaction in systems with strong confinement can enhance the spin–orbit interaction. On the other hand the jumps in the magnetization and following peaks in the susceptibility are clear consequences of the reordering and crossings in the dot energy system provided by the spin–orbit interaction. It is known from the physics of the atomic spectra, that the spin–orbit interaction always provides crossing (or anticrossing) configurations in dependencies of the energy levels on magnetic fields (the general Paschen–Back effect).[40] Therefore, the described effect has the clear physical meaning but the actual magnitude of it should be verified both experimentally and by means of more sophisticated calculations. We have to mention, that it is worth doing because (in contrast to natural atomic systems) quantum dots have an advantage that one can control magnetic properties of the dots by applying external electric fields and changing of the chemical potential.

In summary, we have studied interesting consequences of the spin–orbit interaction in small InAs parabolic quantum dots. The magnetization and magnetic susceptibility of dots with few electrons were calculated. The spin–orbit interaction was involved to control magnetic response of the dots at low temperature. An analog of the general Paschen–Back effect was found for dots with partially filled electronic shells. This property of III–V semiconductor material quantum dots could be useful for the future spintronics research.

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