Spin ordering in semiconductor heterostructures with ferromagnetic δ layers

V. N. Men'shov,[1,2] V. V. Tugushev,[2,3] S. Caprara,[1,4] P. M. Echenique,[1,3] and E. V. Chulkov[1,3]

[1]*Donostia International Physics Center (DIPC), P. de Manuel Lardizabal 4, 20018 San Sebastián, Basque Country, Spain*

[2]*RRC Kurchatov Institute, Kurchatov Square 1, 123182 Moscow, Russia*

[3]*Departamento de Física de Materiales, Facultad de Ciencias Químicas, UPV/EHU and Centro Mixto CSIC–UPV/EHU, Apartado 1072, 20080 San Sebastián, Basque Country, Spain*

[4]*Dipartimento di Fisica, Università di Roma "La Sapienza" and Instituto Nazionale per la Fisica della Materia, SMC and UdR di Roma 1, Piazzale Aldo Moro 2, 00185 Rome, Italy*

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We report on theoretical study of the magnetic properties of a magnetic metal δ layer embedded into a nonmagnetic nondegenerated semiconductor, taking into account the diffusion smearing, that is unavoidable in the case of delta doping. The system of interest is modeled by the δ layer core, enriched in metal atoms, and a nearly depleted smeared periphery. Confinement states in the form of two-dimensional spin-polarized subbands within the semiconductor band gap arise from potential and exchange scattering of carriers at the core. The mechanism of indirect exchange between impurity spins placed within the peripheral region of the δ layer, via partially occupied confinement states, is analyzed. It is shown that, in the case of a ferromagnetic core, the impurity spins align parallel or antiparallel to the core magnetization, due to the polarization of carriers in the confinement states. Allowing for the confinement mechanism of interaction between the impurity spins as well as for the exchange mechanism through deep levels of the semiconductor host, the magnetic configuration of the impurity spins in the peripheral region of the δ layer is obtained in the framework of a phenomenological approach.

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I. INTRODUCTION

Selective alloying appears to be a widespread method to introduce ferromagnetic (FM) ultrathin layers of a magnetic metal (henceforth, δ layers) into a nonmagnetic semiconductor host, when growing hybrid nanostructures of the type semiconductor/ferromagnet. Two such systems are more extensively investigated, which are of interest from the point of view of the fundamental research and of possible practical applications: (1) isolated FM δ layer in semiconductor heterostructure with a quantum well and (2) periodical lattice of FM δ layers within a homogeneous semiconductor [the so-called digital magnetic alloy (DMA)].

While initially the attention was almost exclusively concentrated on structures in which the matrix was realized by III–V semiconductors, an increasing interest was subsequently devoted to systems based on semiconductors of the IV group (Si and Ge). The investigation of semiconductor-ferromagnet heterostructures with an isolated FM δ layer was undertaken in a series of works[1–4] for the GaAs/$\delta\langle$Mn$\rangle$/$Al_xGa_{1-x}As$ layered structures, in which a δ layer of Mn was embedded into a GaAs layer, in the proximity of the GaAs/$Al_xGa_{1-x}As$ interface. Additional doping of the $Al_xGa_{1-x}As$ layer with Be atoms led to the transfer of free carriers (holes) toward the δ layer and allowed to investigate the role of these carriers on FM ordering in the δ layer (the "carrier-mediated ferromagnetism" concept). The study was to a large extent addressed to the achievement of a higher Curie temperature and acceptable transport properties as compared to bulk materials, e.g., diluted magnetic semiconductors (DMSs), such as GaAs:Mn. The results of Refs. 1–4 put in evidence a lot of inconsistencies: even if the Curie temperature exceeded 100 K, at the same time a very small value of the mobility of the free holes was obtained [2–5 $cm^2/(V\cdot s)$]. The low mobility was related with the evident attempt of the authors of Refs. 1–4 to achieve a density of holes as high as possible at the location of the magnetic Mn ions, i.e., at the δ layer. Unfortunately, such a spatial distribution of carriers, alongside with the enhancement of exchange, leads to their strong scattering on ionized Mn impurities, consequently lowering the carrier mobility.

In Refs. 5 and 6 a thorough investigation of the magnetic and transport properties of the GaAs/$\delta\langle$Mn$\rangle$/$In_xGa_{1-x}As$ heterostructure, containing the Mn-rich FM δ layer and the $In_xGa_{1-x}As$ quantum well, spatially separated by a thin GaAs spacer layer, was carried out. Differently from Refs. 1–4, in Refs. 5 and 6 the holes were mostly introduced in the $In_xGa_{1-x}As$ conducting channel rather than in the region of the FM δ layer. The Curie temperature of the system examined in Refs. 5 and 6 was about 40 K, which is somewhat lower than the temperature achieved in Refs. 1–4, but the mobility of the holes was on the order of 10^3 $cm^2/(V\cdot s)$. It was found that an external field induces a magnetic phase transition in the δ layer, accompanied by a biasing of the hysteresis loop of the magnetization. In this way, it was shown that the intentional spatial separation of holes and magnetic atoms not only allows to achieve significant values of the mobility of the carriers in nanostructures of the type semiconductor/ferromagnet but also entails peculiar magnetic properties.

As it is well known, DMSs are characterized by a strong disorder in the distribution of the atoms of magnetic metal in the nonmagnetic semiconductor host. Unfortunately, the equilibrium solubility limit is rather small, the maximum ratio amounting to few atom percent. In contrast to them, DMAs contain discrete layers (monolayers or submonolayers), enriched in magnetic (as a rule, 3*d* transition) metal

atoms, which are regularly embedded into the host. The distance between adjacent magnetic (sub)monolayers is usually on the order of 10 semiconductor layers, which would correspond to a nominal bulk concentration of the metal on the order of 10 at. %. In this respect, DMAs cannot be regarded as some kind of DMSs. Indeed, thanks to the locally high concentration of magnetic atoms, the exchange interaction in a DMA is much stronger than in a DMS with the same nominal concentration of magnetic atoms.

So far, studies on DMAs are far from conclusive, and the quantitative and qualitative understanding of many of their important properties is still lacking. Many DMAs have a higher Curie temperature as compared to DMSs as well as unusual magnetic and magnetotransport properties. For instance, a significant anomalous Hall effect is found even at room temperature, which is a clear evidence for the large spin polarization of carriers. In pioneering works[7,8] the delta doping technique was applied to DMAs based on III–V semiconductors, such as GaAs/Mn and GaSb/Mn. These systems are currently the object of an intense investigation.[9,10] In the GaAs/Mn DMAs, a semiconductor-type conductivity and relatively moderate Curie temperature, about 40 K, were observed,[7] but for the GaSb/Mn DMA, a semi-metal-type conductivity and high Curie temperature exceeding 400 K were reported.[8] Calculations of the electron band structure for these systems indicate peculiar features, such as the spatial localization (confinement) and nearly full spin polarization of carriers in the vicinity of the FM δ layers, the strongly pronounced anisotropy of the magnetic and transport properties,[11] the switching of the interlayer exchange coupling from antiferromagnetic (AFM) to FM with increasing hole concentration.[12] At present, the investigations of DMAs based on semiconductors of the IV group (Si and Ge) are at an initial stage. The first-principles calculations accomplished for the DMAs [Ge/Mn (Ref. 13) and Si/Mn (Ref. 14)] predict sizable carrier polarization at the Mn monolayers and a remarkable redistribution of charge density between the metal monolayers and the semiconductor host. According to Refs. 13 and 14, the interlayer exchange coupling remains FM in the whole ranges of doping and interlayer distance, and the Curie temperature of the (Si,Ge)/Mn digital alloys is higher than that of the (Si,Ge):Mn disordered binary alloys.

The problem of ferromagnetism within the δ layer remains one of the open issues to be investigated from a theoretical point of view. It is unlikely that the δ layer can be treated as a sort of diluted alloy since the magnetic metal atoms are very well localized in a restricted region of the material. Moreover, the mechanism of indirect exchange between local impurity spins via itinerant carriers, that is the standard Ruderman-Kittel-Kasuya-Yosida (RKKY) mechanism transferred from the theory of metal magnetism to the DMS theory,[15] is *a priori* not applicable to nondegenerated magnetic semiconductors, as the systems under discussion frequently are. Evidently, the qualitative interpretation of the results of Refs. 1–4 in the framework of a RKKY-type approach would be possible, provided the δ layer is close enough to the conducting channel.[16] However, the fact that the FM ordering is found in structures where the Mn-rich δ layer inserted into the GaAs nondegenerated host is placed too far from the $In_xGa_{1-x}As$ conducting channel, so that the free carriers (holes) cannot be responsible for the magnetic interaction, casts serious doubts about the validity of the RKKY scheme to describe the system.[5,6] As far as DMAs are concerned, it is apparently irrelevant to use a RKKY-type approach for the explanation of magnetic phenomena in these structures. Indeed, the band-structure calculations[11–14] have demonstrated that in DMAs it is not possible to divide the electron states into localized and itinerant due to their strong (s,p)-d hybridization and to the charge redistribution between the δ layer and the host. The electron spectrum of these systems has a complex structure, which contains both strongly correlated (Hubbard type) narrow bands and weakly correlated wide bands. The FM order, which appears in the δ layer due to the strong electron correlations within the narrow bands, is accompanied by the spin splitting of the wide bands and the formation of the quasi-two-dimensional spin-polarized subbands, in such a way as to lower the total energy of the system in a half-metallic state. Seemingly, the spin ordering in DMAs could be described within a scheme similar to the one adopted for itinerant magnetism in transition metals and their alloys,[17] but the issue is difficult and, to our knowledge, still unsolved.

The multifaceted morphology of the metal δ layer embedded into the semiconductor host puts serious obstacles to the theoretical interpretation of the experimental results on the properties of the delta-doped structures. In fact, the idealized representation of the δ layer as a perfect monolayer or submonolayer of metal atoms regularly embedded into the semiconductor host, on which the aforementioned numerical calculations are based, turns out to be far from the real situation for the reasons listed hereafter.

First, during the synthesis of layered structures, it is impossible to avoid atomic interdiffusion of the various components. Depending on the growing techniques, the diffusion length ranges from several angstroms to several nanometers. In real DMAs, the atoms of the nominally (sub)monoatomic metallic layer undergo diffusion to occupy sites in several neighboring atomic layers of the semiconductor host. The profile of the real metal δ layer, which forms due to the diffusion process, displays a strong gradient along the growth direction of the DMA and could be roughly divided into two different regions: a central region (core layer), which extends over two or three atomic planes enriched in metal atoms; a much broader peripheral region, with locally low dopant concentration, which envelops the core. The peripheral region may be regarded as a DMS. Indeed, as noted in Ref. 18 the [Mn(0.11 nm)/GaAs] DMAs prepared by molecular-beam epitaxy contain heavily doped regions in the vicinity of the Mn core monolayers (lattice planes), in which 80% of Mn is located. At the background level, Mn is also present in the unintentionally doped GaAs interlayer spacers.

Second, in real DMAs, the δ layers have a significantly inhomogeneous morphology in the direction perpendicular to the growth direction. Even under optimal conditions of epitaxial growth with monolayer precision, the thickness of the metal δ layer embedded into the semiconductor host fluctuates with respect to the nominal value on the nanometer scale. One can expect that the compositional integrity of the ultrathin δ layer is not preserved (i.e., the δ layer does not form a continuous metal plane). Thus, nanosized breaches

may appear in the metal plane, and the layer may even be fragmented into separate islands, i.e., nanoislands enriched in metal atoms. In order to interpret the data on the anomalous Hall-effect measurements in the [GaSb/Mn] DMAs with Mn submonolayer insertions, the authors of Ref. 8 supposed that the Mn layer represents a complex quasi-two-dimensional alloy. This alloy consists of both randomly distributed Mn impurities, the spins of which are ferromagnetically ordered below 30–50 K, and the MnSb plane islands, with high Curie temperature, $T_c \approx 580$ K; besides, some Mn atoms migrate into the GaSb host.

Third, the large metal content beyond the equilibrium solubility limit in the semiconductor promotes the phase segregation within the smeared δ layer, possibly with the formation of both magnetic and nonmagnetic inclusions, such as clusters and precipitates, which are nanosized. For example, the DMSs based on IV-group semiconductors doped with Mn show a strong tendency to the formation of secondary phases: the Mn_5Ge_3 and $Mn_{11}Ge_8$ germanates or the Mn_4Si_7 silicides.[19] It is commonly believed that a similar tendency exists in the corresponding DMAs based on Ge or Si, once the Mn concentration exceeds the solubility limit ($\approx 6\%$).

The simultaneous and combined allowance for all the above-mentioned factors makes the set up of an adequate microscopic model for the magnetic ordering in the digital heterostructures, based on semiconductors with embedded FM δ layers, a very complicated task. In this work we undertake the theoretical effort, along the direction indicated above, starting with the study of the magnetic properties of a single FM δ layer inserted into an infinite semiconductor host. In what follows we discuss the semiphenomenological scheme to describe the magnetic ordering in this system, which takes into account only the first of the aforesaid factors, namely, the smearing and spatial inhomogeneity of the δ layer. As it will be evident from further inquiry, the task proves to be highly nontrivial even under such a simplified assumption.

The paper is organized as follows. In Sec. II we discuss the model for a single FM δ layer embedded into a semiconductor host, which includes an ideal FM layer describing the core region and randomly distributed magnetic impurities in the peripheral region. In Sec. III we consider the two-dimensional spin-polarized electron states (confinement states) which are induced by potential and exchange scattering of carriers at the core part of the FM δ layer and determine the dependence of the spin polarization of these states on the distance from the core region. The behavior of the magnetic moment of a single impurity in the peripheral region of the semiconductor host containing the FM δ layer is described in Sec. IV, where we derive the expression for the spin polarization of the carriers in the presence of both the ideal FM δ layer and the impurity spin. In Sec. V we estimate how the FM core influences the indirect exchange coupling between the local impurity moments in the periphery of the smeared δ layer. The possible patterns of magnetic ordering in the periphery are analyzed within an effective functional in Sec. VI. In particular, we describe the structure of the domain wall in the relevant case of AFM ordering within the peripheral region. All calculations are restricted to the zero-temperature limit. Summary and concluding remarks are found in Sec. VII.

II. SET UP OF THE PROBLEM AND MODEL HAMILTONIAN

Let us consider an ultrathin (no more than a few atomic monolayers thick along the axis of growth of the heterostructure, **z**) and homogeneous [on scales larger that the parameter of elementary cell of the host in the (x,y) plane] layer of atoms of the magnetic metal embedded into a nonmagnetic semiconductor host. Assuming that inside the layer FM ordering is present, we call this an ideal FM δ layer. The very assumption of FM ordering is far from obvious. Indeed, due to the strong hybridization of wave functions of semiconductor and metal ions, there exist a sizable redistribution both of charge and spin densities between the host and the δ layer. Strictly speaking, the electron structure and magnetic order of the semiconductor with a (sub)monolayer of magnetic atoms should be studied, for instance, within a microscopic *s-d* Anderson model. Of course, this would require a great deal of numerical calculations. Nevertheless, a simple phenomenological scheme (that we call model of a single FM plane defect) is fairly suited in order to capture, at least qualitatively, the main physical aspects of the system under consideration. Within the model of a FM single plane defect, the FM order in the δ layer, promoted by strong correlations of electron states at the metal ions, is merely postulated. The influence of the FM plane defect on the electron states of the semiconductor host is described by means of an effective one-dimensional potential, which includes both a potential contribution, independent of the spin component, and an exchange contribution, which depends on the spin component. Recently, in Ref. 20 we have fruitfully employed a similar model to calculate the interlayer exchange coupling in DMAs. It may be shown that the present scheme is valid within a static approximation for the self-energy part of the one-particle Green's function in the Anderson model for an ideal FM δ layer.[21]

In the present work we deal with the more realistic situation when the δ layer inserted into the semiconductor host is smeared due to the diffusion of metal atoms into the bulk. The distribution of metal atoms within the δ layer is assumed to be inhomogeneous, so that one can distinguish the thin central part (core) with relatively high concentration of magnetic ions and the thicker external region (periphery) with relatively low concentration of magnetic ions. The core is regarded as an ideal FM δ layer and approximately described by the model of the single FM plane defect. In turn, the periphery represents per se a DMS where rare metal impurity atoms, carrying local spins, are randomly dispersed within the semiconductor host. It should be noted that the nature of the magnetic order which establishes within the peripheral region of the δ layer is *a priori* uncertain. The configuration of impurity spins is governed by competing exchange interactions of different origin and kind; some of them are intrinsic to DMSs, while others are induced by the proximity to the FM core.

It is then necessary to make some additional assumptions. We assume that the local concentration $n(z)$ of magnetic atoms (which occupy random positions $\mathbf{R}_i$ in the semiconductor crystal lattice) is homogeneous in the (x,y) plane of the δ layer and rapidly decays away from it with increasing $|z|$. In

the core region, where the value of $n(z)$ is rather large, there is significant overlap of the wave functions of the magnetic atoms thanks to the hybridization of the electron states at the nearest-neighboring impurity sites. On the contrary, in the periphery, where the value of $n(z)$ is too small, because of the large spatial separation of the magnetic atoms in the alloy, the wave functions belonging to different ions have a negligibly small overlap.

The impurity spin $\mathbf{S}_i$ localized at the site $\mathbf{R}_i=(X_i,Y_i,Z_i)$ experiences a contact exchange interaction with carriers of the semiconductor host. To simplify the treatment, we shall describe the impurity spin $\mathbf{S}_i$ classically, regarding it as a magnetic moment denoted by the same symbol $\mathbf{S}_i$. All the spins are assumed to be of equal magnitude, $|\mathbf{S}_i|=S$. Formally speaking, our approach is correct in the case of a large spin, i.e., within a $1/S$ expansion. Therefore one may hope that the classical approach will not introduce qualitative shortcomings in the estimation of the exchange interaction energy in DMSs.[22] It is clear that, within the given approach, the Kondo screening effect for the impurity spin is ignored. However, the latter restriction is unessential in the case of a nondegenerated semiconductor that is the object under investigation.

We therefore write the Hamiltonian H of the electron states of a nonmagnetic semiconductor in the presence of a FM δ layer in the form

$$H = H_B + H_L + H_I, \tag{1}$$

where

$$H_B = \int d\mathbf{r} \sum_{\alpha} \psi_{\alpha}^{+}(\mathbf{r}) \varepsilon(-i\nabla) \psi_{\alpha}(\mathbf{r})$$

is the Hamiltonian of carriers in the semiconductor host in the absence of the FM δ layer,

$$H_L = \int d\mathbf{r} \sum_{\alpha,\beta} \psi_{\alpha}^{+}(\mathbf{r}) [V\delta_{\alpha\beta} + J(\boldsymbol{\sigma}_{\alpha\beta} \cdot \mathbf{M})] \psi_{\beta}(\mathbf{r}) \delta(z) \tag{2}$$

is the Hamiltonian of interaction between these carriers and the core of the FM δ layer, treated as a FM plane defect, and

$$H_I = \sum_i \int d\mathbf{r} \sum_{\alpha,\beta} \psi_{\alpha}^{+}(\mathbf{r}) \kappa(\boldsymbol{\sigma}_{\alpha\beta} \cdot \mathbf{S}_i) \psi_{\beta}(\mathbf{r}) \delta(\mathbf{r} - \mathbf{R}_i) \tag{3}$$

is the Hamiltonian of interaction between the carriers and the impurity spins in the peripheral region of the δ layer. The operators $\psi_{\alpha}^{+}(\mathbf{r})$ and $\psi_{\alpha}(\mathbf{r})$ create and annihilate an electron with spin projection α onto the quantization axis, at the point $\mathbf{r}=(x,y,z)$. Hamiltonian (2) includes the terms of the potential (V) and exchange $[J(\boldsymbol{\sigma}\cdot\mathbf{M})]$ interaction of carriers with the core, J is the exchange integral, $\mathbf{M}$ is the magnetization of the δ layer, and $\boldsymbol{\sigma}$ is the vector of the Pauli matrices. For the sake of simplicity, we suppose that only the electron states of one band of the semiconductor (for definiteness, say the conduction band) are most strongly affected by the potential of the FM plane defect and give rise to the change in energy of the system. In this work we consider the likely relevant case of a nondegenerated semiconductor, when in the absence of the FM plane defect there are no free carriers, and the Fermi level is located in the band gap of the semiconductor host.

In the vicinity of the FM plane defect, there is some redistribution of the electron density and two-dimensional bound states of carriers (the so-called confinement states) might appear under certain conditions. To describe this effect, we associate an effective attractive potential with the FM plane defect (for electrons of both spin subbands), i.e., we take $V<0$ and $|V|>|J|M$ in Eq. (2). The restriction $|\kappa S| \ll W$ is imposed on the matrix element κ of the exchange interaction of carriers with the impurity spins in Eq. (3) (W is an energy on the order of the conduction-band width) which allows us to avoid at this stage the question about localized states inherent to spin polarons with small radius.

We imply that, in the absence of the metal δ layer, there are no free carriers in the host. The insertion of the δ layer results in a FM plane defect approximately described in our model by the delta-function scattering potential. At the same time, the metal forming the δ layer acts as a donor or an acceptor in the semiconductor host. To correctly describe these two combined effects, strictly speaking, we should solve the rather intricate problem of the self-consistent calculation of both the FM plane effective potential and the position and filling of the electron confinement states split off the band edge by this potential. We shall not deal with this problem. Within our approach, on a phenomenological basis, we merely postulate that the Fermi level lies within the confinement subbands. In other words, all carriers (electrons or holes), which are transferred from the δ layer to the host, occupy the confinement states and not the bulk band states of the semiconductor. Apparently, when the confinement states are empty, the model of a FM plane defect loses its sense. However, it should be noted that the numerical simulations of the band structure in DMAs have established that the confinement states are always partly occupied and spin polarized,[11–14] supporting our phenomenological assumptions.

Below, we study the system at zero temperature. The free energy can be formally written as

$$F = -\frac{1}{\pi} \mathrm{Im} \int d\omega \, \mathrm{Tr} \ln G(\omega), \tag{4}$$

where $G(\omega)=(\omega+i0-H)^{-1}$ is the full Green's function of the semiconductor host in the presence of the smeared δ layer. Following Ref. 22, we express the quantity $\ln G(\omega)$ in terms of the components of the Green's function of the semiconductor host containing only the core part of the δ layer (without the peripheral impurities), $g(\omega)=(\omega+i0-H_B-H_L)^{-1}$, which are diagonal ($g^d$) and off-diagonal ($g^{od}$) with respect to the indexes of the impurity sites $\mathbf{R}_i$. The symbolic form of the corresponding expression is

$$\ln G = \ln g - \ln(1 - g^d \mathbb{K}) + \sum_{n=1}^{\infty} \frac{1}{n} [g^{od} t]^n, \tag{5}$$

where symbol t denotes the single-site scattering matrix that describes the multiple scattering of electrons on the impurity spin placed at the point $\mathbf{R}_i$ within the peripheral region of the δ layer

$$t = \mathbb{K}[\mathbb{I} - g^d\mathbb{K}]^{-1}.$$

By taking into account the spin indexes, the matrix $\mathbb{K}$ is written as $\mathbb{K}_{\alpha\beta}(\mathbf{R}_i) = \kappa(\boldsymbol{\sigma}_{\alpha\beta}\cdot\mathbf{S}_i)$.

According to Eq. (5), the free energy [Eq. (4)] may be divided into three contributions

$$F = F_0 + F_d + F_{od}. \tag{6}$$

The term F_0 is the free energy of the semiconductor host with the ideal δ layer (i.e., the FM plane defect) and it is independent of the electron-impurity interaction. The last two terms in Eq. (6) represent the excess free energy caused by the exchange interaction of carriers with magnetic impurities dispersed in the peripheral region. The site-diagonal term F_d appears in the single-impurity approximation, whereas the site-off-diagonal term F_{od} is related to the interference of the states belonging to different impurity sites. Since we are interested in the situation of a strongly diluted alloy in the periphery of the δ layer, the terms up to the second order of g^{od} will be retained to calculate the energy contribution F_{od}.

III. TWO-DIMENSIONAL SPIN-POLARIZED ELECTRON STATES INDUCED BY AN IDEAL FM δ LAYER

First of all, we wish to draw the attention to the subject of the confinement states, which arise due to the presence of the ideal FM plane defect representing the core of the δ layer. To this purpose, we can neglect the impurities in the peripheral region and write the single-particle Green's function $g_{\alpha\beta}(\mathbf{k},\mathbf{k}',\omega)$ associated with Hamiltonian H_B+H_L in the momentum representation

$$g_{\alpha\beta}(\mathbf{k},\mathbf{k}',\omega) = \delta_{\mathbf{k},\mathbf{k}'}\delta_{\alpha\beta}g^0(\mathbf{k},\omega) + \delta_{\mathbf{k}_\parallel,\mathbf{k}_\parallel'}g^0(\mathbf{k},\omega)T_{\alpha\beta}(\mathbf{k}_\parallel,\omega)g^0(\mathbf{k}',\omega),$$

where the following notations are introduced:

$$T_{\alpha\beta}(\mathbf{k}_\parallel,\omega) = \{[V-(V^2-J^2M^2)\tilde{g}^0(\mathbf{k}_\parallel,\omega)]\delta_{\alpha\beta} + J(\boldsymbol{\sigma}_{\alpha\beta}\cdot\mathbf{M})\} \times [\Delta(\mathbf{k}_\parallel,\omega)]^{-1}, \tag{7}$$

$$\Delta(\mathbf{k}_\parallel,\omega) = [1-V\tilde{g}^0(\mathbf{k}_\parallel,\omega)]^2 - [JM\tilde{g}^0(\mathbf{k}_\parallel,\omega)]^2,$$

$$\tilde{g}^0(\mathbf{k}_\parallel,\omega) = \frac{1}{N_z}\sum_{k_z} g^0(\mathbf{k},\omega) = \int \frac{adk_z}{2\pi} g^0(\mathbf{k},\omega). \tag{8}$$

Here $g^0(\mathbf{k},\omega)=[\omega-\varepsilon(\mathbf{k})]^{-1}$ is the Green's function of the bulk semiconductor, $T_{\alpha\beta}(\mathbf{k}_\parallel,\omega)$ is the full t matrix for the scattering of the band electrons on the FM plane defect, and ω is the frequency. The quasimomentum $\mathbf{k}=(\mathbf{k}_\parallel,k_z)$ is measured from the point where the energy of the conduction band is minimum, $\varepsilon(0)=0$; $\mathbf{k}_\parallel=(k_x,k_y)$ is the component of the quasimomentum parallel to the FM plane defect, a is the lattice parameter of the semiconductor, and N_z is the number of the host sites along the $\mathbf{z}$ direction.

We now proceed to the calculations of the magnetic properties of our model in three steps: first, we show that the FM plane defect may induce bound confinement states and determine their band structure; then, we calculate the explicit expression of the electron Green's function in the presence of the FM plane defect; this expression is finally used to determine the dependence of the spin polarization of the confinement states on the distance from the FM plane defect.

As it is seen from Eq. (8), if $V<0$ (with $|V|>|J|S$), confinement states exist inside the band gap of the host. Their energy spectrum, $\omega=\omega_\pm(\mathbf{k}_\parallel)$, consists of two spin-polarized two-dimensional subbands and is determined by the equation $\Delta(\mathbf{k}_\parallel,\omega)=0$, i.e.,

$$\tilde{g}^0(\mathbf{k}_\parallel,\omega) = (V \pm JM)^{-1}.$$

We adopt henceforth a definite form for the energy spectrum of the host

$$\varepsilon(\mathbf{k}) = \frac{\mathbf{k}^2}{2m} = \frac{\mathbf{k}_\parallel^2}{2m} + \frac{k_z^2}{2m}, \tag{9}$$

where m is the effective mass of an electron near the bottom of the conduction band. Within the adopted effective-mass approximation the dispersion law of the confinement states takes the form

$$\omega_\pm(\mathbf{k}_\parallel) = \omega_\pm + \frac{\mathbf{k}_\parallel^2}{2m},$$

where

$$\omega_\pm = \omega_\pm(0) = -\frac{ma^2}{2}(|V| \pm JM)^2,$$

are the energies of the edges of the corresponding subbands ($\omega_\pm<0$). The quasiparticle excitation energies are small in comparison with the band width $\sim W$, i.e., $|\omega_\pm| \ll W$.

Having determined the energy spectrum of the confinement states, we now proceed to the explicit calculation of the electron Green's function in the presence of the FM plane defect. In the coordinate representation, the Green's function of the confinement states $g_{\alpha\beta}(\omega)$ can be written in the form

$$g_{\alpha\beta}(\mathbf{r},\mathbf{r}',\omega) = g^0(\mathbf{r},\mathbf{r}',\omega)\delta_{\alpha\beta} + \eta_{\alpha\beta}(\mathbf{r},\mathbf{r}',\omega), \tag{10}$$

where

$$g^0(\mathbf{r},\mathbf{r}',\omega) = -\frac{ma^3}{2\pi|\mathbf{r}-\mathbf{r}'|}\exp(-\sqrt{2m|\omega|}|\mathbf{r}-\mathbf{r}'|), \tag{11}$$

$$\eta_{\alpha\beta}(\mathbf{r},\mathbf{r}',\omega) = \frac{m^2a^4}{8\pi^2}\int_0^\infty d\epsilon T_{\alpha\beta}(\epsilon-\omega) \times \frac{\exp[-\sqrt{2m(\epsilon-\omega)}(|z|+|z'|)]}{\epsilon-\omega} \times J_0(\sqrt{2m\epsilon}|\mathbf{r}_\parallel-\mathbf{r}_\parallel'|) \tag{12}$$

and $J_0(\xi)$ is the zeroth-order Bessel function. The t matrix [Eq. (7)] appearing in the integral in Eq. (12) depends on the difference $\epsilon-\omega$ since in correspondence of the band spectrum of the form [Eq. (9)] one finds

$$\tilde{g}^0(\mathbf{k}_\parallel,\omega) = -a\sqrt{\frac{m}{2(\epsilon_{k_\parallel}-\omega)}},$$

where $\epsilon_{k_\parallel}=\mathbf{k}_\parallel^2/2m$ is the energy of the electron motion parallel to the plane of the δ layer.

In view of the forthcoming analysis, it is convenient to put in evidence the potential and exchange spin structure of the function $\eta_{\alpha\beta}(\mathbf{r},\mathbf{r}',\omega)$

$$\eta_{\alpha\beta}(\mathbf{r},\mathbf{r}',\omega) = \eta^{(+)}(\mathbf{r},\mathbf{r}',\omega)[\delta_{\alpha\beta}+(\boldsymbol{\sigma}_{\alpha\beta}\cdot\mathbf{n})] + \eta^{(-)}(\mathbf{r},\mathbf{r}',\omega) \times[\delta_{\alpha\beta}-(\boldsymbol{\sigma}_{\alpha\beta}\cdot\mathbf{n})], \quad (13)$$

where $\mathbf{n}=\mathbf{M}/M$ is the unit vector oriented along the direction of the magnetization of the FM core.

To proceed in the calculation of the dependence of the spin polarization within the confinement states, we need to find the expression of the propagator of the host at equal spatial arguments, $\mathbf{r}=\mathbf{r}'$, bearing in mind that an energy on the order of W must be taken as upper limit for the integration over energies. Then, we obtain

$$g^0(\mathbf{r},\mathbf{r},\omega) = g^0(\omega) = \frac{(a\sqrt{m})^3}{\sqrt{2}\pi}[\sqrt{|\omega|}-\sqrt{W+|\omega|}] \quad (14)$$

and

$$\eta^{(\pm)}(\mathbf{r},\mathbf{r},\omega) = \frac{g^0}{2}\sqrt{\frac{|\omega_\pm|}{W}}\exp(-2|z|\sqrt{2m|\omega_\pm|}) \times E_1[2|z|\sqrt{2m}(\sqrt{|\omega|}-\sqrt{|\omega_\pm|})], \quad (15)$$

where

$$E_1(\xi) = \int_\xi^\infty dt\frac{\exp(-t)}{t} \quad (16)$$

is the exponential integral,[23] $|z|$ is the distance between the point $\mathbf{r}$ in the host and the core, and $g^0=g^0(\omega=0)$.

The exponential integral [Eq. (16)] is a single-valued function in the complex plane cut along the negative real axis. Hence, the imaginary part of $\eta^{(\pm)}(\mathbf{r},\mathbf{r},\omega)$, that is proportional to the local density of states of the corresponding confinement subband, is a steplike function of the frequency, i.e., it vanishes at $\omega<\omega_\pm$ and is finite and constant at $\omega>\omega_\pm$. We note, on passing, that the function $\mathrm{Im}[\eta^{(\pm)}(\mathbf{r},\mathbf{r}',\omega)]$, calculated at arbitrary $\mathbf{r}$ and $\mathbf{r}'$, has similar analytical properties. Indeed, one can obtain the expression

$$\mathrm{Im}[\eta^{(\pm)}(\mathbf{r},\mathbf{r}',\omega)] = \frac{\pi g^0}{2}\sqrt{\frac{|\omega_\pm|}{W}}h(\omega-\omega_\pm)\exp[-\sqrt{2m|\omega_\pm|} \times(|z|+|z'|)]J_0(\sqrt{2m(\omega-\omega_\pm)}|\mathbf{r}_\parallel-\mathbf{r}'_\parallel|), \quad (17)$$

where $h(\omega)$ is the Heaviside function [$h(\omega>0)=1$ and $h(\omega<0)=0$]. Noticeably, the function $\mathrm{Im}[\eta^{(\pm)}(\mathbf{r},\mathbf{r}',\omega)]$ is independent of the frequency when $\mathbf{r}_\parallel=\mathbf{r}'_\parallel$ and oscillates with ω otherwise.

We have now all the ingredients that are needed to determine the spin polarization of the electron states of the semiconductor host in the vicinity of the FM plane defect. Our results are meaningful over distances which exceed essentially the lattice spacing a. To proceed, we calculate the spin polarization of the confinement states induced at the point $\mathbf{r}$ due to the FM plane defect, $\mathbf{m}_0(\mathbf{r})=\mathbf{n}m_0(\mathbf{r})$, where

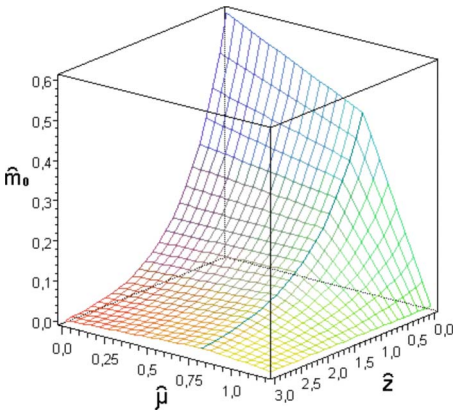

FIG. 1. (Color online) Spin polarization induced by the FM plane defect, Eq. (20), as a function of the distance from the FM plane defect z and of the Fermi energy μ, for $|JM/V|=0.1$. The dimensionless quantities $\hat{m}_0=2W|m_0|[\pi|V|^3(g^0)^2]^{-1}$, $\hat{z}=2ma|Vz|$, and $\hat{\mu}=2|\mu|(ma^2V^2)^{-1}$ are reported on the axes. The thicker line represents the frontier separating the regime where both confinement subbands are occupied, at smaller $\hat{\mu}$, from the regime where a single confinement subband is occupied, at larger $\hat{\mu}$. When $\hat{\mu}$ is large enough, the two subbands are both empty and $\hat{m}_0$ vanishes.

$$m_0(\mathbf{r}) = \mathrm{Im}\int^\mu \frac{d\omega}{\pi}\sum_{\alpha\beta}\sigma^z_{\alpha\beta}g_{\beta\alpha}(\mathbf{r},\mathbf{r},\omega) \quad (18)$$

and we adopted $\mathbf{n}$ as the direction of the local quantization axis. Taking into account Eqs. (15), (17), and (18), one obtains the explicit space dependence of $m_0(\mathbf{r})$ in the form

$$m_0(\mathbf{r}) = m_0^{(+)}(\mathbf{r}) + m_0^{(-)}(\mathbf{r}), \quad (19)$$

where

$$m_0^{(\pm)}(\mathbf{r}) = \pm g^0\sqrt{\frac{|\omega_\pm|}{W}}(\mu-\omega_\pm)h(\mu-\omega_\pm) \times\exp(-2|z|\sqrt{2m|\omega_\pm|}). \quad (20)$$

As it is seen from Eqs. (19) and (20), the carriers of both confinement subbands give rise additively to the spin polarization $\mathbf{m}_0(\mathbf{r})$. The typical behavior of $m_0(\mathbf{r})=m_0(z)$ as a function of the distance from the FM plane defect and of the Fermi energy is shown in Fig. 1. The electron states belonging to the subbands of opposite spin polarization, $\omega_\pm(\mathbf{k}_\parallel)$, have different characteristic lengths near the core, on the order of $l_\pm=(\sqrt{2m|\omega_\pm|})^{-1}$ (with $l_\pm\gg a$). For example, in the case $J<0$, the spin-up subband is characterized by a shorter wavelength as compared to the spin-down subband. As a result, if both subbands are partially occupied, the spin polarization $\mathbf{m}_0(\mathbf{r})=\mathbf{m}_0(z)$ might switch its orientation at the distance $z_0=z_0(\mu)$ from the core, in such a way that $\mathbf{m}_0(\mathbf{r})$ is parallel to $\mathbf{M}$ at $z<z_0$, $\mathbf{m}_0(\mathbf{r})$ is antiparallel to $\mathbf{M}$ at $z>z_0$ (of course, the opposite holds for $J>0$), and $m_0(z_0)=0$. In Fig.

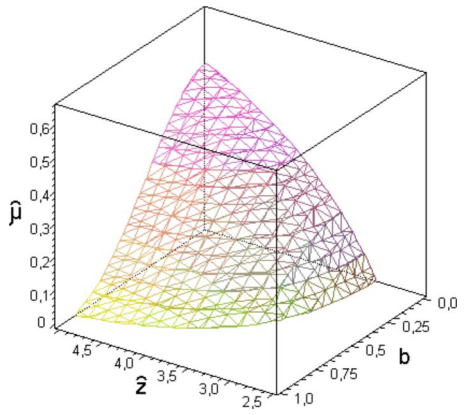

FIG. 2. (Color online) Surface separating the region of parameter space where the electron states are polarized parallel or antiparallel to the magnetization $\mathbf{M}$ of the FM plane defect. The dimensionless quantities $\hat{\mu}=2|\mu|(ma^2V^2)^{-1}$, $\hat{z}=2ma|Vz|$, and $b=|JM/V|$ are reported on the axes. The region underneath the surface $\hat{\mu}=\hat{\mu}(\hat{z},b)$ corresponds to antiparallel polarization for $J<0$ and to parallel polarization for $J>0$. The sign of J dictates the alignment of the spin polarization close to the FM plane defect, which is located at $\hat{z}=0$.

2, we plot surface that separates the region of parameter space where the electron states are polarized parallel or antiparallel to the magnetization $\mathbf{M}$ of the FM plane defect, $z=z_0(\mu,b)$ with $b=|JM/V|$.

IV. SINGLE CLASSICAL SPIN IN A SEMICONDUCTOR HOST WITH AN IDEAL FM δ LAYER

In Sec. III we have studied the formation and spin polarization of the confinement states near the ideal FM plane defect, neglecting the effect of the magnetic impurities in the peripheral region. To include this effect, let us now initially assume that a single classical moment $\mathbf{S}_i$ is inserted into the semiconductor host, which contains the ideal FM δ layer. This magnetic moment produces an additional scattering potential $\kappa(\mathbf{S}_i\cdot\boldsymbol{\sigma})\delta(\mathbf{r}-\mathbf{R}_i)$. The Green function for a particle moving in this system obeys the equation

$$G^{(i)}_{\alpha\beta}(\mathbf{r},\mathbf{r},\omega)=g_{\alpha\beta}(\mathbf{r},\mathbf{r},\omega)+\sum_{\gamma\tau}g_{\alpha\gamma}(\mathbf{r},\mathbf{R}_i,\omega)t_{\gamma\tau}(\mathbf{R}_i,\omega)g_{\tau\beta}(\mathbf{R}_i,\mathbf{r},\omega), \tag{21}$$

where the resolvent $g_{\alpha\beta}(\mathbf{r},\mathbf{r}',\omega)$ is determined by the relations (10)–(15). The single-site scattering matrix $t_{\alpha\beta}(\mathbf{R}_i,\omega)$ in Eq. (21) can be written as

$$t_{\alpha\beta}(\mathbf{R}_i,\omega)=\frac{\kappa(\mathbf{S}_i\cdot\boldsymbol{\sigma})+\kappa^2S^2\breve{g}_{\alpha\beta}(\mathbf{R}_i,\mathbf{R}_i,\omega)}{D(\mathbf{R}_i,\omega)},$$

where

$$D(\mathbf{R}_i,\omega)=\det\left[\delta_{\alpha\beta}-\sum_{\gamma}g_{\alpha\gamma}(\mathbf{R}_i,\mathbf{R}_i,\omega)\kappa(\mathbf{S}_i\cdot\boldsymbol{\sigma}_{\gamma\beta})\right] \tag{22}$$

and the function $\breve{g}_{\alpha\beta}(\mathbf{r},\mathbf{r}',\omega)$ is obtained from the function $g_{\alpha\beta}(\mathbf{r},\mathbf{r}',\omega)$ by means of the formal substitution $\mathbf{n}\to-\mathbf{n}$ in Eq. (13). By definition, the total spin polarization of the confinement states at the point $\mathbf{r}$ is

$$\mathbf{m}(\mathbf{r})=\mathrm{Im}\int^{\mu}\frac{d\omega}{\pi}\sum_{\alpha\beta}\boldsymbol{\sigma}_{\alpha\beta}G^{(i)}_{\beta\alpha}(\mathbf{r},\mathbf{r},\omega)=\mathbf{m}_0(\mathbf{r})+\mathbf{m}_i(\mathbf{r}). \tag{23}$$

This expression includes the component $\mathbf{m}_0(\mathbf{r})$ that is caused by the ideal FM δ layer and was calculated in Sec. III and the component $\mathbf{m}_i(\mathbf{r})$ that is induced by the local scattering potential $\kappa(\mathbf{S}_i\cdot\boldsymbol{\sigma})\delta(\mathbf{r}-\mathbf{R}_i)$. Inserting Eq. (21) into Eq. (23), we obtain

$$\mathbf{m}_i(\mathbf{r})=\mathrm{Im}\int^{\mu}\frac{d\omega}{\pi}\sum_{\alpha\beta\gamma\tau}\boldsymbol{\sigma}_{\alpha\beta}\times g_{\beta\gamma}(\mathbf{r},\mathbf{R}_i,\omega)t_{\gamma\tau}(\mathbf{R}_i,\omega)g_{\tau\alpha}(\mathbf{R}_i,\mathbf{r},\omega). \tag{24}$$

Now, supposing that $\mathbf{r}=\mathbf{R}_j$, we arrive at the expression for the local spin polarization $\mathbf{m}_i(\mathbf{R}_j)$, which is induced at jth impurity site due to the presence of the classical spin $\mathbf{S}_i$ at ith impurity site. Keeping only the lowest order of the perturbation theory in the dimensionless parameter $|\kappa Sg^0|\ll 1$, we arrive at the compact expression

$$\mathbf{m}_i(\mathbf{R}_j)=\mathrm{Im}\int^{\mu}\frac{d\omega}{\pi}\mathrm{Tr}[\boldsymbol{\sigma}g^{od}tg^{od}],$$

where

$$\mathrm{Tr}[\boldsymbol{\sigma}g^{od}tg^{od}]=2\kappa[\mathbf{S}_i(\beta_{ji}\beta_{ij}-\alpha_{ji}\alpha_{ij})+2\mathbf{n}(\mathbf{n}\cdot\mathbf{S}_i)\alpha_{ji}\alpha_{ij}]. \tag{25}$$

Here, the following notations are adopted:

$$\alpha_{ij}=\alpha(\mathbf{R}_i,\mathbf{R}_j,\omega)=\eta^{(+)}(\mathbf{R}_i,\mathbf{R}_j,\omega)-\eta^{(-)}(\mathbf{R}_i,\mathbf{R}_j,\omega), \tag{26}$$

$$\beta_{ij}=\beta(\mathbf{R}_i,\mathbf{R}_j,\omega)=g^0(\mathbf{R}_i,\mathbf{R}_j,\omega)+\gamma(\mathbf{R}_i,\mathbf{R}_j,\omega), \tag{27}$$

$$\gamma_{ij}=\gamma(\mathbf{R}_i,\mathbf{R}_j,\omega)=\eta^{(+)}(\mathbf{R}_i,\mathbf{R}_j,\omega)+\eta^{(-)}(\mathbf{R}_i,\mathbf{R}_j,\omega). \tag{28}$$

For $i\neq j$, Eqs. (11) and (12) are used, whereas Eqs. (14) and (15) are used for $i=j$. Note that $\alpha_{ij}=\alpha_{ji}$ and $\beta_{ij}=\beta_{ji}$.

Within the weak-coupling approximation adopted hereby, $|\kappa Sg^0|\ll 1$, the impurity spin inserted into the semiconductor host does not induce a bound state inside the band gap. In other words, the determinant $D(\mathbf{R}_i,\omega)$ in Eq. (22) does not vanish for all ω and only the occupied confinement states contribute to the integral [Eq. (24)]. As it was already stated, we are assuming that the Fermi energy of the system under consideration, μ, falls within the gap near the conduction-band edge. Substituting the expressions (25)–(28) into Eq. (24), one obtains the spin polarization induced by the impurity spin in the form

$$\mathbf{m}_i(\mathbf{R}_j)=4\kappa g^0\{\mathbf{S}_i[\phi(\mathbf{R}_i,\mathbf{R}_j)+u(\mathbf{R}_i,\mathbf{R}_j)-f(\mathbf{R}_i,\mathbf{R}_j)]+2\mathbf{n}(\mathbf{n}\cdot\mathbf{S}_i)f(\mathbf{R}_i,\mathbf{R}_j)\}, \tag{29}$$

where

$$\phi(\mathbf{R}_i,\mathbf{R}_j)=\frac{1}{g^0}\int^{\mu}\frac{d\omega}{\pi}g^0(\mathbf{R}_i,\mathbf{R}_j,\omega)\mathrm{Im}[\gamma(\mathbf{R}_i,\mathbf{R}_j,\omega)], \tag{30}$$

$$f(\mathbf{R}_i,\mathbf{R}_j)=\frac{1}{g^0}\int^{\mu}\frac{d\omega}{\pi}\mathrm{Re}[\alpha(\mathbf{R}_i,\mathbf{R}_j,\omega)]\mathrm{Im}[\alpha(\mathbf{R}_i,\mathbf{R}_j,\omega)], \tag{31}$$

$$u(\mathbf{R}_i,\mathbf{R}_j)=\frac{1}{g^0}\int^{\mu}\frac{d\omega}{\pi}\mathrm{Re}[\gamma(\mathbf{R}_i,\mathbf{R}_j,\omega)]\mathrm{Im}[\gamma(\mathbf{R}_i,\mathbf{R}_j,\omega)]. \tag{32}$$

The functions $\phi(\mathbf{R}_i,\mathbf{R}_j)$, $f(\mathbf{R}_i,\mathbf{R}_j)$, and $u(\mathbf{R}_i,\mathbf{R}_j)$ are symmetric under permutation of the impurity indexes. As it is seen from Eq. (29), the direction and magnitude of the spin polarization $\mathbf{m}_i(\mathbf{R}_j)$ depend on the mutual orientation of the vectors $\mathbf{M}$ and $\mathbf{S}_i$, on the value and sign of the interaction parameter κ, and on the position of the Fermi level. We point out that Eqs. (30)–(32) are not valid at small distances $|\mathbf{R}_i-\mathbf{R}_j|\lesssim(mW)^{-1/2}$ within the effective-mass approximation.

The relation (29) between the spin polarization $\mathbf{m}_i(\mathbf{R}_j)$ and the spin $\mathbf{S}_i$ allows us to define the linear-response coefficients, namely, the longitudinal susceptibility and transverse susceptibility, such that $\mathbf{m}_i^{\parallel}(\mathbf{R}_j)=\chi_{ij}^{\parallel}\kappa\mathbf{S}_i$ and $\mathbf{m}_i^{\perp}(\mathbf{R}_j)=\chi_{ij}^{\perp}\kappa\mathbf{S}_i$. The longitudinal susceptibility then reads

$$\chi_{ij}^{\parallel}=\chi_{ji}^{\parallel}=4g^0[\phi(\mathbf{R}_i,\mathbf{R}_j)+u(\mathbf{R}_i,\mathbf{R}_j)+f(\mathbf{R}_i,\mathbf{R}_j)] \tag{33}$$

and the transverse susceptibility reads

$$\chi_{ij}^{\perp}=\chi_{ji}^{\perp}=4g^0[\phi(\mathbf{R}_i,\mathbf{R}_j)+u(\mathbf{R}_i,\mathbf{R}_j)-f(\mathbf{R}_i,\mathbf{R}_j)]. \tag{34}$$

These quantities will be used in Sec. V to express the exchange coupling between peripheral impurities

Both the spin polarization [Eq. (29)] and the susceptibilities [Eqs. (33) and (34)] are rather complicated functions of the space coordinates, whose expressions could be found only numerically, in the general case. In the asymptotic limit, $\sqrt{2m|\mu|}R_{ij}\gg 1$, where $R_{ij}=|\mathbf{R}_i-\mathbf{R}_j|$, we find

$$\chi_{ij}^{\parallel}\simeq\chi_{ij}^{\perp}\simeq 4g^0\phi(\mathbf{R}_i,\mathbf{R}_j),$$

$$\begin{aligned}\phi(\mathbf{R}_i,\mathbf{R}_j)=&\frac{|g^0|}{2mR_{ij}^2}\frac{|\mu|}{W}\exp(-\sqrt{2m|\mu|}R_{ij})\\&\times\left\{\frac{|\omega_-|}{W}\exp[-\sqrt{2m|\omega_-|}(|Z_i|+|Z_j|)]\right.\\&\times J_0(k_-^{\parallel}\rho_{ij})h(\mu-\omega_-)\\&+\frac{|\omega_+|}{W}\exp[-\sqrt{2m|\omega_+|}(|Z_i|+|Z_j|)]\\&\left.\times J_0(k_+^{\parallel}\rho_{ij})h(\mu-\omega_+)\right\}.\end{aligned} \tag{35}$$

Here, $\rho_{ij}^2=(X_i-X_j)^2+(Y_i-Y_j)^2=R_{ij}^2-(Z_i-Z_j)^2$ and $k_{\pm}^{\parallel}=\sqrt{2m(\mu-\omega_{\pm})}$. Therefore, the asymptotic behavior of the spin polarization induced by an isolated impurity in the peripheral region of the δ layer is

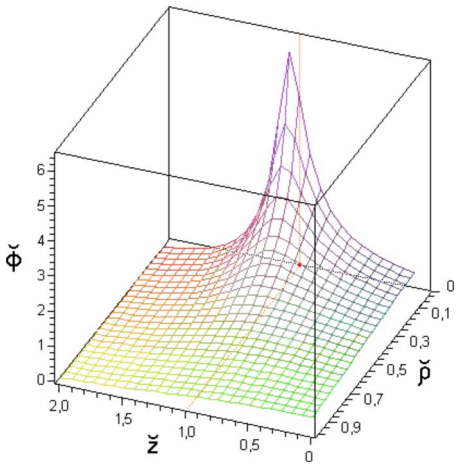

FIG. 3. (Color online) Spin polarization of the electron states induced by an isolated magnetic impurity in the peripheral region of the δ layer, Eq. (36). The dimensionless variables $\breve{z}=\sqrt{2m|\omega_+|}z$, $\breve{\rho}=\sqrt{2m|\omega_+|}\rho_{ij}$, and $\breve{\phi}=2\pi\sqrt{2W}\exp(2Z_i\sqrt{2m|\omega_+|})(m^{3/2}\omega_+^2)^{-1}\times\phi(\mathbf{R}_i,\mathbf{R}_j)$, where $\phi(\mathbf{R}_i,\mathbf{R}_j)$ is taken from Eq. (30), are reported on the axes. The FM plane defect is located at $\breve{z}=0$. The figure illustrates the case when the impurity is located at $\breve{z}=1$ and $\breve{\rho}=0$. This point is shown in the figure. The function $\phi(\mathbf{R}_i,\mathbf{R}_j)$ is formally plotted for $\breve{\rho}\geq 0.1$.

$$\mathbf{m}_i(\mathbf{R}_j)\approx 4\kappa g^0\phi(\mathbf{R}_i,\mathbf{R}_j)\mathbf{S}_i. \tag{36}$$

The expressions (35) and (36) demonstrate the oscillating distribution of the spin density around the local impurity moment in the plane parallel to the δ layer core. The periods of oscillation of the contributions of the two confinement subbands are proportional to the inverse of the corresponding Fermi wavevectors, $k_{\pm}^{\parallel}$. The oscillations are exponentially damped by the prefactor $\exp(-\sqrt{2m|\mu|}R_{ij})$, whose characteristic length is generically shorter than the oscillation wavelength. A typical behavior of the spin density induced by an isolated impurity in the periphery of the δ layer is shown in Fig. 3.

V. INFLUENCE OF THE CORE ON THE ORDERING OF THE LOCAL SPINS IN THE PERIPHERY OF A SMEARED FM δ LAYER

In Secs. III and IV we have determined the spin polarization of the electron states which are formed near an ideal FM plane defect and the influence of isolated peripheral magnetic moments on such a polarization. Now, we want to analyze the interaction mechanism between peripheral magnetic moments, in the presence of the ideal FM plane defect.

In the smeared FM δ layer the magnetic metal atoms located at the core are coupled via the indirect exchange interaction with atoms of the same metal situated in the peripheral region at fairly large distance from the core. The point is that the magnetic bias field of the core, whose influence is transferred by means of the confinement electron states, affects the peripheral magnetic atoms. To clarify this peculiar proximity effect in the framework of our model, we need to calculate the diagonal contribution F_d to the free energy [Eq. (6)]. Let us write it in the explicit form

$$F_d = \sum_i \mathrm{Im} \int^{\mu} \frac{d\omega}{\pi} \ln D(\mathbf{R}_i, \omega) \tag{37}$$

with

$$D(\mathbf{R}_i, \omega) = 1 - 2\kappa(\mathbf{n}\cdot\mathbf{S}_i)\alpha_{ii} + \kappa^2 S^2(\alpha_{ii}^2 - \beta_{ii}^2).$$

In the case of the nondegenerated semiconductor host, the integral [Eq. (37)] is nonvanishing provided at least one of the confinement subbands is partially occupied, i.e., $\omega_+ < \mu < 0$. Omitting the terms independent of the mutual orientation of the vectors $\mathbf{n}$ and $\mathbf{S}_i$ and, hence, immaterial in the present context, with an accuracy up to the terms on the order of $(\kappa S g^0)^2$, we obtain for the exchange part of the diagonal free energy the expression

$$F_d^{(ex)} = \sum_i [A_i^{(1)}(\mathbf{n}\cdot\mathbf{S}_i) + A_i^{(2)}(\mathbf{n}\cdot\mathbf{S}_i)^2], \tag{38}$$

where the exchange integrals are given by

$$A_i^{(1)} = A^{(1)}(\mathbf{R}_i) = 2\kappa \int^{\mu} \frac{d\omega}{\pi} \mathrm{Im}[\alpha(\mathbf{R}_i, \mathbf{R}_i, \omega)],$$

$$A_i^{(2)} = A^{(2)}(\mathbf{R}_i) = 4\kappa^2 \int^{\mu} \frac{d\omega}{\pi} \mathrm{Im}[\alpha(\mathbf{R}_i, \mathbf{R}_i, \omega)] \times \mathrm{Re}[\alpha(\mathbf{R}_i, \mathbf{R}_i, \omega)]$$

and the expression for the function $\alpha(\mathbf{R}_i, \mathbf{R}_i, \omega)$ has been given above, see Eq. (26).

The first, bilinear, term in Eq. (38) is proportional to the spin polarization of the carriers in the confinement states at the impurity site, $A_i^{(1)} = 2\kappa m_0(\mathbf{R}_i)$. The magnitude of the coupling depends on the position of the Fermi level and on the distance between the impurity site and the core, $A_i^{(1)} = A^{(1)}(|Z_i|, \mu)$. When only one of the confinement subbands (say, the spin-up subband) is occupied, the effective indirect exchange integral $A_i^{(1)}$ keeps the same sign at all the impurity sites. This means that, if the local exchange constants J and κ have the same sign, $J\kappa > 0$, the impurity spins in the periphery $\{\mathbf{S}_i\}$ are polarized in the direction parallel to the core magnetization $\mathbf{M}$; similarly, if $J\kappa < 0$, the impurity spins are polarized in the direction antiparallel to the vector $\mathbf{M}$. However, when both the spin-up and the spin-down confinement subbands are occupied, the exchange integral $A_i^{(1)}$ changes sign at $|Z_i| = z_0(\mu)$, following the coordinate dependence of the electron-spin polarization $\mathbf{m}_0(z)$, Eqs. (19) and (20). Hence, the alignment of the impurity spins near the core, at $|Z_i| < z_0(\mu)$, is opposite to the alignment of the impurity spins far off the core, at $|Z_i| > z_0(\mu)$. In this case, one could say that the magnetic impurity atoms in the periphery would screen to a certain extent the core magnetization of a smeared (realistic) FM δ layer.

The second, biquadratic, term in Eq. (38) can be expressed via the exponential integral [Eq. (16)]. Under the conditions $\sqrt{|\omega_\pm|}/W \ll 1$ and $2|Z_i|\sqrt{2m}(\sqrt{|\omega_\pm|} + \sqrt{|\mu|}) \gg 1$, we obtain the estimate

$$A_i^{(2)} \sim \frac{\omega_\pm}{W}(\kappa g^0)^2 \frac{\exp[-2\sqrt{2m}(\sqrt{|\omega_\pm|} + \sqrt{|\mu|})|Z_i|]}{(2\sqrt{2m}|Z_i|)^2}.$$

It is clear that, as a rule, the bilinear coupling dominates over the biquadratic coupling, $|A_i^{(1)}| \gg |A_i^{(2)}|$. Nevertheless, when both the confinement subbands are occupied, the role of the biquadratic coupling could turn out to be important for the impurity atoms placed at the distance $|Z_i| \approx z_0(\mu)$ from the core, where the magnitude of $A_i^{(1)}$ is very small.

To determine the indirect exchange coupling between the impurity magnetic atoms dispersed in the peripheral region of the smeared FM δ layer, one has to calculate the off-diagonal contribution to the free energy [Eq. (6)], F^{od}. By keeping the terms up to the second order in g^{od}, we obtain the expression

$$F_{od} = -\sum_{ij} \mathrm{Im} \int^{\mu} \frac{d\omega}{2\pi} \mathrm{Tr}[g^{od} t g^{od} t] = -\sum_{ij} \mathrm{Im} \int^{\mu} \frac{d\omega}{2\pi} \sum_{\alpha\beta\gamma\tau} g_{\alpha\beta}(\mathbf{R}_i, \mathbf{R}_j, \omega) \times t_{\beta\tau}(\mathbf{R}_j, \omega) g_{\tau\gamma}(\mathbf{R}_j, \mathbf{R}_i, \omega) t_{\gamma\alpha}(\mathbf{R}_i, \omega), \tag{39}$$

which takes into account all paired interactions between the impurity local spins, $i \neq j$. The off-diagonal Green's function g^{od} entering Eq. (39) is given in Eqs. (11) and (12), if one sets $\mathbf{r} = \mathbf{R}_i$ and $\mathbf{r}' = \mathbf{R}_j$, where i and j are the impurity site indexes ($i \neq j$). Below we omit the terms that are independent of the mutual orientation of the moments of the impurities and the core, $\mathbf{S}_i$, $\mathbf{S}_j$, and $\mathbf{M}$, and therefore are irrelevant to the determination of the exchange coupling.

To the second order in the expansion parameter $\kappa S g^0$, the exchange part of the integrand in the right-hand side of the Eq. (39) is given by

$$\mathrm{Tr}[g^{od} t g^{od} t]|_{ex} = 2\kappa^2[(\mathbf{S}_i\cdot\mathbf{S}_j)(\beta_{ij}\beta_{ji} - \alpha_{ij}\alpha_{ji}) + 2(\mathbf{n}\cdot\mathbf{S}_i) \times (\mathbf{n}\cdot\mathbf{S}_j)\alpha_{ij}\alpha_{ji}]. \tag{40}$$

Correspondingly, the energy of the indirect exchange interaction between the magnetic atoms in the periphery takes the form

$$F_{od}^{(ex)} = \sum_{ij} [B_{ij}(\mathbf{S}_i\cdot\mathbf{S}_j) + C_{ij}(\mathbf{n}\cdot\mathbf{S}_i)(\mathbf{n}\cdot\mathbf{S}_j)]. \tag{41}$$

The exchange integrals can be expressed via the nonlocal susceptibility [Eqs. (33) and (34)]

$$B_{ij} = -\frac{\kappa^2}{2}\chi_{ij}^{\parallel}, \tag{42}$$

$$C_{ij} = -\frac{\kappa^2}{2}(\chi_{ij}^{\parallel} - \chi_{ij}^{\perp}). \tag{43}$$

Note that values of B_{ij} and C_{ij} decay exponentially with increasing separation between the impurity atoms and the core of the δ layer over the scales on the order of $l_\pm = (\sqrt{2m|\omega_\pm|})^{-1}$, since the indirect interaction appears in the nondegenerated semiconductor host due to the quasiparticle excitations through the energy barrier $|\omega_\pm|$ separating the

confinement states from the conduction-band edge. At small values of the ratio $|\omega_{\pm}|/W$, the main contribution to the exchange energy [Eq. (41)] comes from the first term involved in the integral B_{ij}. It is noteworthy that B_{ij} does not vanish even at $\mathbf{M}=0$.

VI. COMPETITION BETWEEN DIFFERENT KINDS OF EXCHANGE INTERACTIONS AND MAGNETIC ORDERING IN THE PERIPHERY OF A SMEARED FM δ LAYER

In Sec. V we have determined the interaction between the peripheral spin and the core of a smeared δ layer, and the indirect exchange between the peripheral spin mediated by the confinement states. Now, we want to discuss the possible patterns of spin configurations in the peripheral region.

The contributions [Eqs. (38) and (41)] to the exchange energy of the local moments are associated with the carrier confinement at the core of the δ layer. However, when analyzing the magnetic ordering in the periphery of a FM δ layer, other possible sources of exchange interaction should be considered. Indeed, we recall that, according to our model, the peripheral region of the δ layer constitutes per se a nondegenerated DMS. In such a medium, the superexchange interaction between the local moments through the deep impurity states in the host plays an important role. For instance, this matter had been investigated in detail in Ref. 24. Since deep impurity states were neglected in the initial Hamiltonian (1), we introduce an additional phenomenological term of the Heisenberg type to the free energy of the system, $F_{SE}=\Sigma_{ij}I_{ij}(\mathbf{S}_i\cdot\mathbf{S}_j)$, where the exchange integral I_{ij} depends only on the intersite distance $|\mathbf{R}_i-\mathbf{R}_j|$, but not on the separation of the moments $\mathbf{S}_i$ and $\mathbf{S}_j$ from the core. The details of the band structure of the semiconductor host determine the sign of the coupling I_{ij}. Thus the whole expression for the exchange energy of the impurity local moments in the periphery of the δ layer can be cast in the form

$$F^{(ex)}=\sum_i [A_i^{(1)}(\mathbf{n}\cdot\mathbf{S}_i)+A_i^{(2)}(\mathbf{n}\cdot\mathbf{S}_i)^2]+\sum_{ij}[B_{ij}(\mathbf{S}_i\cdot\mathbf{S}_j) + C_{ij}(\mathbf{n}\cdot\mathbf{S}_i)(\mathbf{n}\cdot\mathbf{S}_j)]+\sum_{ij} I_{ij}(\mathbf{S}_i\cdot\mathbf{S}_j). \quad (44)$$

The case $I_{ij}<0$ is not of deep interest, since the superexchange (last) term in Eq. (44) merely enhances the tendency to FM ordering, which exists due to the confinement (first two) terms in Eq. (44). Conversely, in the situation $I_{ij}>0$, that is quite possible according to Ref. 24, the AFM superexchange coupling could prevail in the periphery far away from the core, where the integrals $A_i^{(1,2)}$, B_{ij}, and C_{ij} are exponentially suppressed. Hence, the competition between the superexchange and the confinement mechanisms of coupling of the local moments is expected to appear in the periphery, not too far from the FM core. Unfortunately, a thorough analysis of the magnetic configurations for the system [Eq. (44)] is very difficult because of the complicated dependence of the exchange integrals $A_i^{(1,2)}$, B_{ij}, C_{ij}, and I_{ij} on the site coordinates $\{\mathbf{R}_i,\mathbf{R}_j\}$ of the randomly distributed impurities. Therefore, we restrict our analysis to a qualitative estimate of the possible magnetic states of the model [Eq. (44)], under the condition $I_{ij}>0$, adopting some simplifying assumptions.

First, we assume that only the lower (say, spin-up) confinement subband is partially occupied and the terms proportional to $A_i^{(2)}$ and C_{ij} are negligibly small, after the smallness of the parameter $\sqrt{|\omega_{\pm}|/W}\ll 1$. Hereafter we omit the superfluous superscript and let $A_i^{(1)}\to A_i$. Second, carrying out the double summation in Eq. (44), we retain the paired interactions only between the nearest-neighboring impurity moments, $\langle ij\rangle$. Moreover, the average interimpurity distance, $\bar{a}\sim\bar{n}^{-1/3}$, is regarded to be much shorter than the characteristic smearing thickness of the δ layer, L, the carrier wavelength, and the confinement state scale, so that the relations $\bar{a}\ll l_+,(k_+^{\|})^{-1}\ll L$ hold. This means that, in the periphery of the δ layer, a rather large number of sites of the host are substituted by the impurity atoms, and the concept of the average impurity concentration, $\bar{n}$, is meaningful. Within this approximation, the integral I_{ij} does not depend on the site indexes ($I_{ij}\to I$) and, in turn, the integrals A_i and B_{ij} depend only on the distance between the core and the impurity site(s). Thus, Eq. (44) is reduced to the expression

$$F^{(ex)}=\sum_i A_i(\mathbf{n}\cdot\mathbf{S}_i)+\sum_{\langle ij\rangle}[B_{ij}+I](\mathbf{S}_i\cdot\mathbf{S}_j), \quad (45)$$

where the summation in the second term is carried out over the indexes of the nearest-neighboring sites $\langle ij\rangle$

$$A_i\approx -A\exp\left(-\frac{|Z_i|}{l_+}\right), \quad (46)$$

$$B_{ij}\approx -B\exp\left(-\frac{|Z_i|+|Z_j|}{l_+}\right) \quad (47)$$

with $A,B,I>0$.

Let us introduce the impurity concentration $n(z)$ averaged over a scale larger than $\bar{a}$, which is homogeneous in the (x,y) plane, symmetric, $n(z)=n(-z)$, and decays away from the core in the $\mathbf{z}$ direction. We first evaluate the energy of the system [Eqs. (45)–(47)] for the simplest inhomogeneously ordered configuration of the impurity moments. Namely, we imagine that, within a layer adjacent to the core, at $0<|z|<L_0/2$, a homogeneous FM phase is established, and within two layers that are further away from the core, at $L_0/2<|z|<L/2$, a homogeneous two-sublattice AFM phase exists. The magnetizations of the FM layer and of the core are parallel to each other; the magnetizations of the AFM sublattices are coplanar to the vector $\mathbf{M}$. In the mean-field approximation, the exchange energy per unit of area, $f^{(ex)}$, for this configuration is given as a function of the thickness L_0 by the expression

$$f_{F/A}^{(ex)}(L_0)=\int_0^{L_0/2}dzn(z)\left[dIS^2-(dBS^2+2AS)\exp\left(-\frac{2z}{l_+}\right)\right] - \int_{L_0/2}^{\infty}dzn(z)\left[dIS^2-dBS^2\exp\left(-\frac{2z}{l_+}\right)\right]. \quad (48)$$

The parameter d is a coordination number that depends on

the distribution of the impurity atoms among the sites of the host at the periphery. Under the assumption of an uncorrelated distribution of the impurity atoms among the sites of a simple cubic lattice, one can take the rough estimate $d \approx 6$.

When the peripheral region of the smeared δ layer has a fairly sharp boundary, the impurity concentration can be approximated by the steplike function, $n(z)=\bar{n}h(L-2|z|)$. In this case Eq. (48) is reduced to the form

$$f_{F/A}^{(ex)}(L_0) = -\bar{n}\frac{dS^2}{2}\left\{ I(L-2L_0) + Bl_+\left[1+\exp\left(-\frac{L}{l_+}\right) - 2\exp\left(-\frac{L_0}{l_+}\right)\right] + \frac{2Al_+}{dS}\left[1-\exp\left(-\frac{L_0}{l_+}\right)\right]\right\}.$$

If $dBS+A<dIS$, the function $f_{F/A}^{(ex)}(L_0)$ reaches its minimum value at $L_0=L_0^{(min)}=0$. In other words, the AFM ordering dominates practically over the whole periphery. However, if $dBS+A>dIS$, the function $f_{F/A}^{(ex)}(L_0)$ has a minimum at a nonzero thickness $L_0=L_0^{(min)}<L$, with

$$L_0^{(min)} = l_+ \ln\left(\frac{BdS+A}{IdS}\right). \tag{49}$$

Under such conditions, the mixed FM/AFM state appears to be preferred for the impurity moments in the periphery.

Consider, for example, the situation in which the exchange between the impurity moments via the confinement electron states gives the main contribution to the FM ordering within the layer $|z|<L_0/2$ and the polarization effect of the moments under the influence of the "molecular" field $\mathbf{n}A_i$ associated to the core is comparably weaker. As the parameter (A/BdS) tends to zero, one has $L_0^{(min)}=0$ for $I>B$, and $L_0^{(min)}=l_+\ln(B/I)$ for $I<B$. This situation might be met in the case of a δ layer with weakly FM or even nonmagnetic core. When the superexchange through the deep electron states is strong, $I>B$, the dispersed local moments in the peripheral region of the smeared δ layer align antiferromagnetically, and the FM order could be present only within the core. On the contrary, when the superexchange is weak, $I<B$, a more complex magnetic configuration establishes, which includes a FM region near the core and an AFM region far off it.

It is remarkable that we arrive at the same results if we adopt a smooth concentration distribution of the form $n(z)=n(0)\exp(-|z|/z^{(0)})$.

Our rough estimations on the basis of the functional [Eq. (48)] qualitatively sketch out the ordering pattern of the impurity moments. The simplified scheme discussed above shows that the spin density in the vicinity of a real δ layer may be of an inhomogeneous nature, with domains of both FM and AFM arrangement of the impurity moments. However, it is evident that the real magnetic structure in the periphery is by no means realized in the form of a FM and an AFM layers with a sharp boundary between them. The competition among various types of exchange coupling in the periphery would lead to appearance of a spatially inhomogeneous state of the type of a domain wall.[25] The characteristic length scale and nature of the domain wall is determined by the exchange stiffness and magnetic anisotropy of the DMS. In the mean-field model of the δ layer with competing interactions, where the FM exchange between the impurity local moments prevails over the AFM exchange near the core and exactly the opposite situation occurs in the periphery, a domain wall parallel to the plane of the δ layer mainly describes the large-scale arrangement of the impurity moments.

To capture the key features of the spatial magnetic structure of the δ layer, we need to make some simplifications. On the one hand, we assume that the thickness of the FM domain $\sim L_0$ is rather small as compared to the characteristic length scale of the spatial variation in the spin density, ζ, which is implied to be comparable to (or lesser than) the length scale of the smearing of the δ layer L. On the other hand, we assume that the exchange stiffness within the FM region (i.e., the exchange stiffness of the core) is by order of magnitude larger than the stiffness within the AFM periphery. We neglect the occurrence of perpendicular domain walls in the FM core region (which could appear, for instance, due to dipole-dipole interaction). Then, we restrict the core magnetization and the peripheral spin-polarization density to lay parallel to the plane of the δ layer and be uniform along this plane. Making these assumptions, we can now study the magnetic ordering of the δ layer by means of an effective one-dimensional model which includes an infinitesimally thin and exchange hard FM layer inserted into an exchange soft AFM bulk.

The total free-energy functional per unit area of this system is written as a sum of the free energy of the AFM region, $f_A^{(ex)}$, the fourfold anisotropy contribution, f_{an}, and the free energy of the interface between the FM layer and the AFM bulk, f_{int},

$$f = f_A^{(ex)} + f_{an} + f_{int}.$$

In the absence of the FM layer, every lattice plane of impurity magnetic atoms in the bulk of the assumed two-sublattice antiferromagnet is regarded as fully compensated which is quite natural in the situation of the random alloy in the periphery. Therefore, far from the FM layer, the impurity local moments align along one of the easy axes of anisotropy, but approaching the FM plane defect, the magnetizations of the AFM sublattices deviate from this axis under the influence of the exchange anisotropy field at the interface.

The first step to describe the magnetic configuration is to go from a discrete array of impurity magnetic-moment vectors to a continuous magnetization field. This is done in the usual way by replacing the moment vector $\mathbf{S}_i$ at the site i by the continuous variable $\mathbf{S}(z)$. As stated above, for simplicity, we neglect variations in the magnetizations parallel to the plane of the δ layer so that the field $\mathbf{S}(z)$ depends only on the argument z. The interaction terms between moments at neighboring impurity sites in Eq. (45) are dealt with by assuming that $\mathbf{S}(z)$ changes slowly over length scales on the order of the lattice spacing. The sublattice magnetizations are identified by unit vectors $\boldsymbol{\alpha}(z)$ and $\boldsymbol{\beta}(z)$. The energy in the AFM bulk is

$$f_A^{(ex)} = \int dz \left\{ \Lambda\left[\left(\frac{d\boldsymbol{\alpha}}{dz}\right)^2 + \left(\frac{d\boldsymbol{\beta}}{dz}\right)^2\right] + \Delta\boldsymbol{\alpha}\cdot\boldsymbol{\beta}\right\}, \tag{50}$$

where $\Delta=dIS^2\bar{n}$. The exchange energy terms are constructed by expanding the magnetization fields about neighboring im-

purity sites. The exchange stiffness constant in the AFM bulk has been defined as $\Lambda = dIS^2\bar{n}^{1/3}$ to include the material parameters, such as the coordination number and the impurity concentration. The interface exchange energy per unit area is then written as

$$f_{int} = -jS\mathbf{M}\cdot(\boldsymbol{\alpha}+\boldsymbol{\beta}).$$

The exchange integral j can be defined as an average measure of the coupling between the spin density of the FM core and the moments of the AFM sublattices in the periphery. The vector $\mathbf{M}$ is directed along one of the easy axes, for definiteness, say the $\mathbf{x}$ axis. Using an angular representation for the sublattice magnetizations

$$\boldsymbol{\alpha} = [\sin(\theta+\varphi),\cos(\theta+\varphi),0],$$

$$\boldsymbol{\beta} = [\sin(\theta-\varphi),\cos(\theta-\varphi),0],$$

the total energy can be written as the functional

$$f[\theta,\varphi] = \int dz\Bigg\{2\Lambda\left[\left(\frac{d\theta}{dz}\right)^2+\left(\frac{d\varphi}{dz}\right)^2\right]+\Delta\cos(2\varphi) + 2K[\sin^2(2\theta)\cos^2(2\varphi)+\cos^2(2\theta)\sin^2(2\varphi)] - 2jSM\delta(z)\cos(\varphi)\sin(\theta)\Bigg\}, \quad (51)$$

where $K = K_0\bar{n}$ is the fourfold anisotropy constant.

The extrema of the energy are found by varying the functional $f[\theta,\varphi]$ with respect to each angle. However, we restrict ourselves to configurations symmetric with respect to the $\mathbf{x}$ axis, i.e., $\theta = \pi/2 = \text{const}$ and $\varphi(\pm\infty) = \pi/2$, and $\frac{d\varphi}{dz}(\pm\infty) = 0$. The impurity moment density is determined only by the angle φ, which measures the deviation of the orientation of the AFM sublattice magnetization from the direction of the core magnetization $\mathbf{M}$ (see Fig. 4). The minimum deviation is reached at $z=0$. The variation $\frac{\delta f}{\delta\varphi}=0$ results in the differential equation

$$\Lambda\frac{d^2\varphi}{dz^2}+\frac{\Delta}{2}\sin(2\varphi)-K\sin(4\varphi)=0 \quad (52)$$

with the associated boundary condition

$$\frac{d\varphi}{dz}(0+)-\frac{d\varphi}{dz}(0-)=\frac{jSM}{2\Lambda}\sin\varphi(0). \quad (53)$$

The existence of the first integral of Eq. (52) allows us to obtain the exact solution in the form

$$\varphi(z) = \arccos\left[\sqrt{\frac{4\lambda}{(1-k^2)(1+\lambda^2)+2(1+k^2)\lambda}}\right], \quad (54)$$

where

$$\lambda = \lambda(z) = \exp\left[\frac{4}{k}\sqrt{\frac{K}{\Lambda}}(|z|+z_b)\right] \quad (55)$$

and

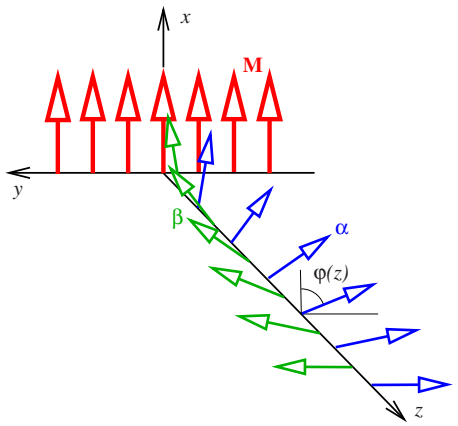

FIG. 4. (Color online) Schematic pattern of the domain wall which is formed parallel to the plane of the δ layer [the (x,y) plane in the figure], in the case of AFM ordering of the impurity spins in the peripheral region. The case $\lambda(0)-1 \ll 1$ is illustrated, in which the two-sublattice magnetizations $\boldsymbol{\alpha}(z)$ and $\boldsymbol{\beta}(z)$ are both aligned nearly parallel to the core magnetization $\mathbf{M}$ in the proximity of the core [where $\varphi(0)\approx 0$] and the ideal Néel structure with antiparallel sublattice magnetizations [$\varphi(0)\approx\frac{\pi}{2}$] is only recovered far off the core.

$$k^2 = \frac{4K}{4K+\Delta}.$$

The constant z_b is determined by the boundary condition (53). Equations (54) and (55) describe the pattern of the domain wall of a two-sublattice AFM in a local magnetic field. In the limit of a strong coupling between the FM and AFM subsystems, when

$$\lambda(0)-1 \approx \frac{16\sqrt{K\Lambda}}{jSMk} \ll 1$$

the dependence $\varphi(z)$ takes the form of a 90° domain wall, $\varphi(0)\approx 0$ and $\varphi(\pm\infty)=\pi/2$ (see Fig. 4): the two magnetization are nearly parallel to each other (and to the core magnetization $\mathbf{M}$) near the core and become antiparallel (and perpendicular to the core magnetization $\mathbf{M}$) away from the core, where the ideal Néel AFM structure is recovered. In the opposite case

$$\sqrt{\lambda(0)} \approx \frac{16\sqrt{K\Lambda}}{jSMk\sqrt{1-k^2}} \gg 1$$

the sublattice magnetizations deviate only slightly from the $\mathbf{y}$ easy axis perpendicular to the vector $\mathbf{M}$

$$\varphi(z) = \frac{\pi}{2}-\frac{jSMk}{8\sqrt{K\Lambda}}\exp\left(-\frac{2}{k}\sqrt{\frac{K}{\Lambda}}|z|\right),$$

i.e., the AFM order in the peripheral region is of a nearly ideal Néel type even in the proximity of the core. As mentioned above, the characteristic length scale of the spatial variation in the magnetization density $\varphi(z)$ does not exceed the scale of the smearing of the δ layer, $\zeta = \frac{k}{2}\sqrt{\frac{\Lambda}{K}} \ll L$.

Substitution of the solutions (54) and (55) into Eq. (51) yields the energy of the system

$$f = f_0 + \Delta \sqrt{\frac{\Lambda}{K}} \left\{ \frac{4k}{(1-k^2)[1+\lambda^2(0)] + 2(1+k^2)\lambda(0)} \times \left[1 - \frac{4\lambda(0)}{1-k^2} \frac{\lambda(0)+1}{\lambda(0)-1} \right] - \ln \left| \frac{\lambda(0) + \frac{1-k}{1+k}}{\lambda(0) + \frac{1+k}{1-k}} \right| \right\}, \quad (56)$$

where $f_0 = -L\Delta$ is the energy of the two-sublattice antiferromagnet in the Néel state. As it is seen from Eq. (56), it is energetically more favorable to form a parallel domain wall in the AFM periphery and lower the exchange energy at the FM/AFM boundary rather than to align the AFM moments along the easy axis and keep the maximum frustration of the exchange couplings at this boundary.

VII. SUMMARY AND CONCLUDING REMARKS

The extent and character of the interaction between the FM δ layer and quasiparticles in the semiconductor host are the key problems in the physics of the delta-doped nanostructures. The explanation of their properties is directly connected with both the morphology of the δ layer and the spin polarization of carriers over the whole doped region. The matter is still poorly studied both from the experimental and the theoretical point of view.

Thereupon, we wish to draw attention to Ref. 18, mentioned in Sec. I, in which the spin polarization of carriers in the epitaxial heterostructure [Mn(0.11 nm)/GaAs] was explored by hot-electron photoluminescence. It was shown that holes in the Mn δ layers and electrons in the GaAs spacers experience the strong influence of the FM core layer. The magnitude of the spin polarization of these carriers is proportional to the magnetization of the δ layer. In Ref. 26 a strong enhancement in electroluminescence intensity and a high degree of its circular polarization (up to 50% at low temperature, $T=1.8$ K, and magnetic field $B=9$ T) are reported in Schottky diodes with near contact InGaAs/GaAs quantum well and a Mn δ layer. High values of the degree of polarization of electroluminescence are suggested to be due to effective exchange interaction of holes with magnetic moments of Mn atoms in the nearby δ layer. Using the results of Sec. III, we can attempt a comparison with experimental data and estimate the value of the characteristic length of the confinement states. Within the assumption that only one confinement subband is occupied (say, the spin-up subband) and that the degree of polarization of electroluminescence found in Ref. 26 is proportional to the spin density $m_0(\mathbf{r})$ in Eq. (20), calculated at the InGaAs/GaAs heterocontact, we obtain for this length scale the estimate $l_+ \approx 50$ Å, which holds within logarithmic accuracy (see Fig. 5). We point out that, to better interpret the data of Ref. 26, the distance from the core should not be estimated as the thickness d_s of the GaAs spacer, i.e., the distance between the InGaAs channel and the nominal location of the Mn δ layer, but rather as the difference $d_s - d_c$, where $d_c \approx 2$ nm is the characteristic length of the diffusion smearing of the δ layer (i.e., the core half width). Of course, a shift by the constant quantity $-d_c$ does not affect the result of the exponential fit of the tail of the data, i.e., the value of l_+.

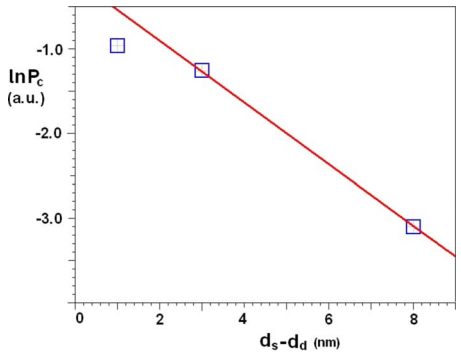

FIG. 5. (Color online) Comparison between experimental data (Ref. 26) (boxes) and our theoretical prediction (solid line). The experimental data represent the logarithm of the normalized difference between the degree of polarization of the electroluminescence signal and the background reference value, as a function of the distance from the δ layer in Schottky diodes with near contact InGaAs/GaAs quantum well and a Mn δ layer [adapted from Ref. 26]. The degree of polarization P_c is taken in correspondence of the magnetic field $B=9$ T, where the electroluminescence signal is nearly saturated.

From the value of l_+ we can extract an estimate for the position of the edge of the lower confinement-state subband, $|\omega_+| = (2ml_+^2)^{-1} \approx 0.01$ eV, where the value $m \approx 0.1m_0$ has been used. In turn, from the relation $|V| = 2|\omega_+| l_+/a$, we obtain for the binding potential of the FM plane defect the estimate $|V| \approx 0.25$ eV, where the value $a \approx 5$ Å has been used. The exchange part of the interaction between the carriers and the core can be roughly estimated by order of magnitude, in analogy with DMSs, as $|JM/V| \approx 0.1-0.2$.

As we discussed above, in Sec. I, the field and temperature dependence of the magnetization of GaAs/$\delta\langle$Mn$\rangle$/GaAs/$\mathrm{In}_x\mathrm{Ga}_{1-x}$As/GaAs quantum wells with the $\delta\langle$Mn$\rangle$ layer separated from the well by a 3-nm GaAs spacer were studied in the temperature range of 3–300 K in a magnetic field up to 6 T.[6] A phase transition to a FM state induced by an external magnetic field was found to occur at a temperature below 40 K with a magnetization hysteresis loop shifted from zero magnetic field. Our model of coexisting FM and AFM regions within the smeared δ layer, developed in Secs. IV and V, provides a microscopic basis for the exchange-biasing phenomenological scheme adopted in Ref. 6 to interpret the outcomes of the experiments.

In our opinion, nontrivial experimental results showing how the delta doping exerts influence upon magnetic properties of a DMS were obtained in Ref. 27. The hysteresis loops obtained in the $(\mathrm{Ga}_{1-x}\mathrm{Mn}_x)$N thin films with $x=0.009$ at $T=5$ K indicated a remarkable (by an order of magnitude) increase in the magnetization once the Mn δ layer had been inserted into the GaN buffer layer at a distance of 25 nm from the $(\mathrm{Ga}_{1-x}\mathrm{Mn}_x)$N/GaN interface. Nevertheless, in the delta-doped GaN film, ferromagnetism was not observed.[27] Reference 28 reported on the preparation of delta-doped amorphous Ge:Mn films, which displayed rather peculiar magnetic and magnetoresistance features, depending on the Mn concentration and on the nominal distance between metal layers. These results were explained under the assumption that there exist FM regions of the secondary phase, with

high Curie temperature, which appeared to be antiferromagnetically coupled with each other at low temperature. The authors of Ref. 29, by means of molecular-beam epitaxy, succeeded in manufacturing a perfect [Si(20 Å)/Mn(x)] multilayers with the nominal δ layer thicknesses $x=1$, 1.5, and 2.0 Å. The samples exhibited, on the one hand, FM ordering above room temperature and, on the other hand, a Curie temperature decreasing with increasing Mn content.

The up-to-date state of the theoretical achievements does not still permit to satisfactorily interpret the experimental data on hybrid nanostructures based on semiconductors with ultrathin FM metal layers. Above all, it would be necessary to concentrate the effort on the description of the magnetic ordering in a structurally inhomogeneous layer. For instance, the way in which the alloy disorder influences FM ordering in the metal submonolayer could be accounted for by means of the coherent potential approximation. It seems that the question about the magnetic properties of the layer with the nanosized islandlike or clusterlike morphology is of current relevance as well. As far as the problem of the magnetic polaron in the nondegenerated semiconductor materials under consideration is concerned, this remains a greatly controversial topic. The issue is beyond the scope of our paper. Nonetheless, we would like to point out that, according to the very concept of magnetic polaron,[30] the exchange interaction between local impurity spins in the nondegenerated DMS is mediated by electron jumps through states of the bulk impurity band. To leave this mechanism of exchange out of our model, we can formally suppose that the impurity band (if any) lies far from the confinement bands and the Fermi level and, hence, does not contribute to the exchange.

Thus, we presented a semi-phenomenological scheme to describe the spin ordering in the system containing an ultrathin FM metal layer embedded into a nondegenerated semiconductor host. The diffusion smearing of this layer is modeled by its partitioning into two regions with relatively high and low content of magnetic ions, i.e., the core and the periphery, respectively. We analyzed two types of a proximity effect: (1) the polarization of the local spins of the metal ions in the periphery induced by the FM core and (2) the indirect exchange coupling among these spins via the core. Both effects owe their appearance to the electron confinement states inside the semiconductor energy gap, which are inherent to the potential of a FM plane defect in the bulk host. Having determined the exchange integrals, we constructed the effective Hamiltonian of the local spins and estimated the energies of some magnetic configurations of the system.

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