Localized states in 2D semiconductors doped with magnetic impurities in quantizing magnetic field

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A theory of magnetic impurities in a 2D electron gas quantized by a strong magnetic field is formulated in terms of Friedel-Anderson theory of resonance impurity scattering. It is shown that this scattering results in an appearance of bound Landau states with zero angular moment between the Landau subbands. The resonance scattering is spin selective, and it results in a strong spin polarization of Landau states, as well as in a noticeable magnetic field dependence of the $g$ factor and the crystal field splitting of the impurity $d$ levels.

I. INTRODUCTION

Unique properties of two dimensional electron systems (2DES) in strong magnetic fields together with their potential applications in microelectronics put these systems among the hottest topics in the studies of strongly correlated electron systems. The fractional quantum Hall effect is the brightest manifestation of unusual quantum statistics of 2DES (see, e.g., Ref. [1]). Yet, even in the case of an integer occupation an extremely rich variety of excitations can be observed in these systems. Various types of excitons [2–4] and collective topological excitations (skyrmions) [5,6] arise due to interplay between orbital and spin degrees of freedom.

Impurity scattering is responsible for broadening of Landau levels and creation of localized states in a 2DES. The genesis of the bound states due to a short-range potential scattering was described in Refs. [7,8]. However, the role of magnetic impurities in formation of the excitation spectrum in 2DES was not discussed thoroughly as yet. Meanwhile, the recent experimental achievements in doping semiconductors with magnetic impurities in confined geometries are significant. A high enough concentration of transition metal (TM) impurities is inserted in heterostructures formed by several III-V and II-VI semiconductor compounds [9]. For example, in II-VI heterostructures (Cd,Mn)Te/(Cd,Mg)Te planar concentration of Mn is comparable with the 2D electron concentration (see, e.g., [10,11]). Apparently, in such cases TM is the dominant impurity that predetermines the filling of the gaps between the Landau levels. To describe modifications of the energy spectrum of a 2DES one should first consider the problem of an isolated magnetic impurity in a 2D electron gas in a strong quantizing magnetic field. This problem is solved in the present paper.

Our study of magnetic impurities in a 2DES is based on two existing approaches: (i) we generalize the theory of TM impurities developed for the bulk semiconductors and summarized in Refs. [12,13]; (ii) we show that the behavior of TM impurities has much in common with the properties of isoelectronic point-like impurities, and in a sense our theory is a generalization of the approach formulated in Refs. [7,8] for the case of spin selective resonance impurity scattering that results in an appearance of bound Landau states between the bare Landau levels. We find also that the interplay between the orbital and spin degrees of freedom results in a significant modification of the $g$ factors both of the impurity $d$ electrons and electrons on the bound Landau levels.

II. IMPURITY LEVELS AND BOUND STATES IN 2DES

Perturbation inserted by TM impurities in a magnetic field quantized energy spectrum of electrons in semiconductors can be described by a Friedel-Anderson resonance scattering model (see, e.g., [13]). According to this model, TM impurity introduces its 3d-level either in the semiconductor energy gap or in the nearest valence or conduction band (depending on the atomic number of the impurity). As a result, the scattering amplitude due to the local impurity potential acquires a strong energy dependence, characteristic of the Friedel-type resonance scattering. A quantizing
magnetic field makes the electron motion finite in a plane perpendicular to the field direction. Only those electron orbitals are perturbed by the impurity potential, which envelop the defect cell. Therefore, the degeneracy of each Landau level in a 2DES is partially lifted by the impurity scattering. A similar problem was discussed earlier for the case of potential scatterers in a quantizing magnetic field (see, e.g., \[\text{[2,7,8,14]}\]). Here we study the case of resonance scattering in the 2DES, which is formed, e.g in GaAs/GaAlAs semiconductor heterostructures.

The calculation starts from the impurity Hamiltonian in a magnetic field $B$ parallel to the $z$-axis,

$$H_c = H_0 + V_d(r - R_0)$$  \hspace{1cm} (1)

where

$$H_0 = \frac{1}{2m^*} \left( \mathbf{P} + \frac{e}{c} \mathbf{A} \right)^2 + V(z)$$  \hspace{1cm} (2)

describes the motion of an electron in the conduction band with the effective mass $m^*$, confined in the $z$ direction by the potential $V(z)$. $V_d(r - R_0)$ is the substitutional impurity potential at a site $R_0$. The effect of the periodic lattice potential is taken into account in the effective mass approximation. It may be applied since we are interested in the properties of magnetically quantized states near the bottom of the lowest conduction band. The behavior of the impurity wave functions and the positions of the impurity levels are predetermined by the singularities in the spectrum of these states. Therefore, we neglect in our calculations the contributions of the higher conduction bands as well as those of the valence bands. Then the band wave functions assume the form

$$\Psi_{\lambda,j}(r) = \Phi_{\lambda}(\rho, \phi)\chi_j(z).$$  \hspace{1cm} (3)

Here $\lambda$, $j$ are the quantum numbers describing the finite electron motion in the $xy$-plane and in the $z$-direction, respectively. $\chi_j(z)$ are eigenfunctions of the confining potential $V(z)$. Only one state of this confining potential closest to the electron Fermi level will be taken into account in what follows. The corresponding index $j$ will be suppressed below. It is also convenient for our purposes to describe the electron motion in the $xy$-plane by means of the cylindrical coordinates $\rho$, $\varphi$. We choose the cylindrical gauge for the vector potential $\mathbf{A} = (-\frac{1}{2}B, \frac{1}{2}B, 0)$. Then $\lambda = nm$ where $n$ is the Landau level index and $m$ is the orbital quantum number enumerating the states within a given Landau level. The planar component of the wave function (3) has the form

$$\Phi_{nm}(\rho, \phi) = C_{nm} L_{n + \frac{|m|}{2}}^{|m|/2}(\xi) e^{-im\varphi}e^{-\frac{\rho^2}{2\zeta}},$$  \hspace{1cm} (4)

$$\rho = l_B \sqrt{2\xi}, \quad l_B^2 = \frac{h^2}{eB},$$

$$C_{nm} = \frac{(n + \frac{m - |m|}{2})!}{2\pi l_B^2 (n + \frac{m + |m|}{2})!} (n \geq \pm m \geq -\infty).$$

Here $E_n = \frac{\hbar^2}{2m^*} \frac{2n + 1}{l_B^2}$ is the energy of the $n$-th Landau level, $L_{n + \frac{m - |m|}{2}}^{|m|/2}(\xi)$ is Laguerre polynomial.

In accordance with the general scheme of the resonance model [3], the wave function of an electron, localized in a discrete impurity level, is represented by an expansion

$$\Phi_{\gamma\mu} = F_d^\gamma \varphi_{\gamma\mu} + \sum_{\lambda} F_\lambda^\gamma \varphi_{\lambda}. $$  \hspace{1cm} (5)

The atomic $d$-orbital $\varphi_{\gamma\mu}$ forms the "core" of the impurity wave function that retains its 3D character, because its radius $r_d$ is small in comparison with the width of the well $V(z)$ responsible for the confinement in the $z$ direction. Here $\gamma = e$, $t_2$ determines the irreducible representation of the crystalline point group for the $d$ states, $\mu$ enumerates lines of these irreducible representations. The orbital effect of the magnetic field is negligible on the atomic scale. The crystal field splitting of the energy levels,

$$\varepsilon_\gamma = \varepsilon_d + \langle \gamma\mu|W|\gamma\mu \rangle,$$  \hspace{1cm} (6)

is the only effect of the crystalline environment. Here

2
\[ W(\mathbf{r} - \mathbf{R}_0) = \sum_{j \neq 0} U_h(\mathbf{r} - \mathbf{R}_j) \]

is the crystal field of the neighboring host ions in the lattice sites \( \mathbf{R}_j \) acting on the impurity \( d \)-electrons. The "tail"

\[ \Phi_{b\gamma\mu} = \sum_{\lambda} F_{\lambda}^{\gamma\mu} \varphi_{\lambda} \]

of the impurity wave function \( \Phi_{b\gamma\mu} \) is a superposition of the wave functions \( \varphi_{\lambda} \) with \( \lambda = nm \), which are obtained by orthogonalizing the functions \( \Phi_{b\gamma\mu}(r) \) to the \( d \) states. This tail falls down at large distances, \( \Phi_{b\gamma\mu}(r) \sim r^{-1} \exp(-\kappa_r r) \).

A rough estimate of the localization parameter is \( \kappa_{\gamma} \approx \hbar^{-1} \sqrt{2m_e|E_{i\gamma}|} \) where \( |E_{i\gamma}| \) is the depth of the impurity level relative to the nearest Landau subband. A detailed discussion of the asymptotic behavior of the impurity wave functions for bulk semiconductors can be found in the book [13]. Due to the obvious symmetry of the problem it will be convenient for the future analysis to choose the origin of the system of coordinate coinciding with the impurity.

Substitution of the wave function (6) into the Schrödinger equation with the Hamiltonian (1) results in the system of equations for the expansion coefficients \( \{ F_{\lambda}^{\gamma\mu}, F_{d}^{\gamma\mu} \} \),

\[ (\varepsilon_{\gamma} - E) F_{d}^{\gamma\mu} + \sum_{\lambda} \langle \gamma \mu | V_d | \lambda \rangle F_{\lambda}^{\gamma\mu} = 0, \]

\[ (E_{\lambda} - E) F_{\lambda}^{\gamma\mu} + \langle \lambda | V_d | \gamma \mu \rangle F_{d}^{\gamma\mu} + \sum_{\lambda'} \langle \lambda' | V_d | \lambda \rangle F_{\lambda'}^{\gamma\mu} = 0 \]

(\( E_{\lambda} \equiv E_n \)). The system of equations (7) may be represented in the matrix form (see, e.g., [15])

\[ \begin{pmatrix} B & -V^T \\ -V & D \end{pmatrix} \begin{pmatrix} b \\ d \end{pmatrix} = 0 \]  

where

\[ (b, d) = (F_{\lambda}^{\gamma\mu}, F_{d}^{\gamma\mu}) \]

and \( T \) denotes the transposition of the matrix. The elements of the matrices \( B, D, V \) are

\[ B_{\lambda,\lambda'} = (E - E_{\lambda}) \delta_{\lambda,\lambda'} - \langle \lambda | V_d | \lambda' \rangle, \]

\[ D_{\gamma\mu,\gamma'\mu'} = (E - \varepsilon_{\gamma}) \delta_{\gamma,\gamma'} \delta_{\mu,\mu'}, \]

\[ V_{\gamma\mu,\lambda} = \langle \gamma \mu | V_d | \lambda \rangle, \]

respectively. The energy levels are determined by the secular equation for the system (8)

\[ \det M \equiv \det (D(E) - VB^{-1}(E)V^T) = 0. \]

It follows from Eq. (10) that the energies of the impurity bound states are determined by the equation

\[ E - \varepsilon_{\gamma} - M_{\gamma}(E) = 0, \]

where

\[ M_{\gamma}(E) = \sum_{\lambda\lambda'} \frac{\langle \gamma \mu | V_d | \lambda \rangle \langle \lambda | Q^{-1} | \lambda' \rangle \langle \lambda' | V_d | \gamma \mu \rangle}{E - E_{\lambda}}, \]

\[ Q = 1 - VG, \quad G = (1 \cdot E - H_0)^{-1}, \]

1 is the unit matrix.

Eq. (11) is the basic equation of the theory. It describes the renormalization of both the impurity \( d \)-level \( E_{i\gamma} \) and of the Landau bands \( E_{\lambda} \). The self energy part \( M_{\gamma}(E) \) contains information about the potential scattering [13]. In
particular, the zeros of the matrix $Q(E)$ determine the Landau levels modified by the short range impurity potential $\langle \lambda | V_d | \lambda \rangle = V$. Since $V_d$ is nonzero mostly within the impurity crystalline cell, the dependence of its matrix elements on the indices of the Landau states is very weak, and we neglect it for the sake of simplicity. Just this very type of the potential is used in the theory of the point-like impurity scattering [7,8]. This potential contains a bound $d$-level so it is responsible both for the resonance and potential impurity scattering (see [15] for more details). The sign of the potential scattering amplitude depends on specific characteristics of the substitutional impurity atom relative to those of the substituted host atom. It can be either negative or positive.

Bound impurity states in case of a potential scattering with $V < 0$ were investigated in Refs. [7,8]. In order to use the results of those studies it is convenient to represent the matrix $M = V \tilde{G} V$ in a more symmetric form

$$M = V \tilde{G} V.$$

Here $\tilde{G}(E)$ is the Green function of a single short range impurity problem found in [7]. Now the matrix element $M_{\gamma \lambda}(E_{i\gamma})$ acquires the form

$$M_{\gamma \lambda}(E_{i\gamma}) = \sum_{\beta} \frac{\langle \gamma \mu | V_d | \beta \rangle \langle \beta | V_d | \gamma \mu \rangle}{E_{i\gamma} - E_\beta}.$$  \hspace{1cm} (13)

where $|\beta\rangle$ stand for the eigenfunctions of magnetic field quantized electrons in the local potential $V_d$,

$$|\beta\rangle = Q^{-1}|\lambda\rangle.$$

The most important property of this solution is that all the states $|nm\rangle$ with nonzero angular momenta ($m \neq 0$) are left intact by the short range potential $V_d$ because they have nodes at the impurity site. Thus, $E_\beta = E_\lambda$ for the states with $m \neq 0$ [3]. This is true also for the resonant scattering potential, although in this case the statement is only approximate. The matrix elements

$$\langle nm| V_d | \gamma \mu \rangle \sim \left( \frac{\rho_d}{l_B} \right)^{|m|} \prec 1$$

for $m \neq 0$, since the typical localization radius $\rho_d$ of the impurity d-functions is much smaller than the magnetic length $l_B$. It means that only one d-orbital, $|1\rangle \propto |r^2 - 3z^2\rangle \sim Y_{20}$, may be strongly hybridized with states with $m = 0$. Thus, both potential and resonance components of the TM impurity act on the same cylindrically symmetric states, meaning that only the states with $m = 0$ enter the self energy [13]. We use the Green function in Eq. (13) in the form

$$\tilde{G}(\xi, z; \xi', z') = \sum_n \frac{\varphi_b(\xi; E_n) \chi(z) \varphi^*_b(\xi'; E_n) \chi^*(z')}{E - E_{bn}}.$$ \hspace{1cm} (14)

where only the bound states with $m = 0$, belonging to the relevant quantum level $E_j$ of the confinement potential $V(z)$, are retained. The energy spectrum and the wavefunctions of these states were calculated in ref. [7]. Several results of this paper, which we need for the further discussion, are presented below.

The wavefunctions $\varphi_b(\xi; E_{bn})$ for the bound Landau states with $m = 0$ have the following asymptotic at large $\xi$,

$$\varphi_b(\xi, E_{bn}) = \frac{\Gamma(\frac{1}{2} - \alpha_n)}{\sqrt{2\pi \psi(\frac{1}{2} - \alpha_n)}} \frac{W_{\alpha_n,0}(\xi)}{l_B^{\frac{1}{2}}}. $$ \hspace{1cm} (15)

Here $\alpha_n = \frac{1}{2} (1 - \epsilon_{bn} l_B^2)$, $\epsilon_{bn} = 2m \pm E_{bn}/\hbar^2$, $W_{\alpha_n,0}(\xi)$ is the Whittaker function, $\psi(\alpha_n)$ is the digamma function. The energy levels $\epsilon_{bn}$, split from the corresponding Landau levels $\epsilon_{n0}$, are described by the following equation,

$$\psi(\alpha_n) + \ln \frac{2}{|\epsilon_i| l_B^2} = 0.$$ \hspace{1cm} (16)

where $E_i$ is the energy level of an electron, bound by the impurity attractive potential $V$ at $B = 0$.

The first bound state appears below the bottom of the conduction band. Its energy is given by the equation

$$\epsilon_{b0} = \epsilon_i - \frac{1}{6\epsilon_i l_B^2},$$ \hspace{1cm} (17)
which follows from Eq. (14), provided the energy level \( E_i \) is deep enough (or the magnetic field is weak), \( |\varepsilon_{bi}| \gg \hbar^2 B^2 \).

Other discrete levels in this case are slightly shifted Landau levels. It follows from (16) that

\[
\varepsilon_{bn} = \varepsilon_{n-1,0} + 2l_B^{-2} \ln \frac{2e^{\psi(a_n)}}{|\varepsilon_i|l_B^2}. 
\]  

(18)

With an increase of the magnetic field the impurity level \( \varepsilon_{n} \) moves upward towards \( \varepsilon_{n0} \).

The positions of the Landau bound states induced by the resonance scattering component of the impurity potential are determined by the self energy part

\[
M_e(E) = \sum_n \frac{|V_{en}|^2}{E - E_{bn}}. 
\]  

(19)

Therefore, Eq. (11) becomes

\[
E_{i\sigma} - \varepsilon_{\sigma} = M_e(E_{i\sigma}) 
\]  

(20)

(we restored the \( d \)-electron spin indices for the reasons, which will be explained in the next section). Here the matrix elements

\[
V_{en} = \int d^3r \, \varphi_{e1}(r)V_d(r)\varphi_b(\xi, E_{bn})\chi_0(z) 
\]  

(21)

describe the hybridization of the atomic and bound Landau states. They are magnetic field dependent (see Section 4 for further discussion).

Two lowest solutions of Eq. (20) arise below the first Landau level. To illustrate the mechanism of the renormalization we neglect all the Landau levels in this equation except for the lowest one, described by Eq. (17). Then two first discrete levels follow from the simplified equation,

\[
(E_{i\sigma}^{(b,a)} - \varepsilon_{\sigma})(E_{i\sigma}^{(b,a)} - E_{i0}) = |V_{eb}|^2. 
\]  

(22)

If the resonance \( d \)-level arises deep below the quantized band level \( E_{n=0} \), then the bonding state \( E_{i\sigma}^{(b)} \) is the renormalized impurity \( e \)-level and the antibonding state \( E_{i\sigma}^{(a)} \) is the former localized level \( E_{i0} \) shifted upwards. In this case the resonance scattering is weak, and it cancels partially the contribution of the short range potential \( V_d \). If the resonance level appears above \( E_{i0} \), then the (now bonding) level \( E_{i\sigma}^{(b)} \) deepens in comparison with the level \( E_{i0} \).

The qualitative graphical solution of Eq. (20) is presented in Fig. 1.

Fig. 1a exhibits a graphical solution of Eq. (14) in the general case. Here two lowest solutions correspond to the states \( E_{i\sigma}^{(b,a)} \), and all the remaining solutions represent the states with \( m = 0 \) split from the degenerate Landau levels \( E_{i0} \). In fact, all these states are solutions of Eqs. (14) or (18) shifted upward. Fig. 1b illustrates graphical solution of simplified secular equation (24).

It is known \( [13] \) that the resonance level \( E_{i\sigma} \) of TM impurities in a neutral state with configuration \( 3d^n \) always arises below the bottom of the conduction band. However, in the case of charged impurity states \( 3d^{n+1} \) the bare \( e \)-level may appear very close to the bottom of the conduction band. For example, vanadium impurity \( V^{2+} \) in GaAs possesses just this kind of spectrum \( [12] \). In some cases (e.g., Cr in GaAs) the \( e \)-state of the charged impurity may appear above the bottom of the conduction band \( [13] \), and this is the case of a strong resonance scattering, leading to a shift of the levels \( E_{bn} \) downward (dashed line in Fig. 1a). A further discussion of possible experimental realizations of the strong resonance impurity scattering is presented in the following sections.

Since \( 3d \)-impurity interacts only with the band orbitals in its nearest vicinity, one should take into account the scatter in the positions of the Landau levels in different parts of the sample due to long range fluctuations of the local fields. This scatter is described by a Gaussian distribution, so the split-off levels with \( m = 0 \) form a replica of this distribution. As a result, in real samples one should observe the density of states presented in Fig. 2.

The removal of the symmetry selection rules for the \( e \)-states also influences significantly the crystal field splitting \( \Delta_{CF} = E_{i\sigma 2} - E_{i\sigma e} \) of the impurity levels. For example, in the particular case of the charged \( V^{2+} \) impurity in GaAs the level \( E_{ie} \) is shifted down due to repulsion from the bound state, whereas the influence of the quantizing magnetic field on the level \( E_{i\sigma 2} \) is negligible. As a result we expect an increase of \( \Delta_{CF} \) due to the Landau quantization. A similar effect of the spatial quantization on the crystal field splitting of TM impurities in semiconductor quantum wells was discussed in \( [17] \).
FIG. 1. (a) Graphical solution of Eq. (20) for bound impurity and Landau states in case of the $de$-level below the quantized Landau grid (the solid $E - \varepsilon_e$ line) and in case of the $de$-level within the Landau grid (the dashed $E - \varepsilon_e$ line). (b) Graphical solution of Eq. (22) for the bound impurity and Landau states.
III. SPIN STRUCTURE OF LOCALIZED LEVELS

It is shown above that the resonance scattering does not change radically the orbital part of the localized states formed by the purely potential impurity scattering. However, taking into account the spin structure of the impurity states results in more significant distinctions between simple isoelectronic and TM impurities in quantizing magnetic fields. In the latter case the influence of TM impurity on Landau levels is spin selective.

To demonstrate this selectivity, one should take into account the fact that the resonance states described by Eq. (5) belong to the impurity 3d-shell with a definite configuration of electron spins [13]. Let us consider, for example, the state of a TM impurity in a configuration \( d^n \) where the last \( (n - \text{th}) \) electron occupies the bonding level \( E_i\sigma \) (22).

Then the many-electron state of the 3d shell may be represented as

\[
d^n = \left( n e_1^{r_1} e_2^{r_2} t_3^{r_3} t_4^{r_4} \right) \sum_{r_i=n}.
\]

This notation means that the impurity has \( n \) electrons in its 3d shell, where \( r_1 \) and \( r_2 \) electrons with spin up and down, respectively, are in the \( e \)-states, \( r_3 \) and \( r_4 \) electrons with spin up and down, respectively, are in the \( t \)-states.

Normally, TM ions in a crystal field of III-V semiconductors exist in the so called high spin state, which means that the \( t_{2\sigma} \) - and \( e_{\sigma} \) - states are occupied in accordance with the Hund rule. Therefore, the spins of the \( e \) electrons in the 3d\(^n\) ions with \( n \leq 5 \) (from Ti to Mn) are directed parallel to the external field \( B \). These electrons form the deep energy levels \( E_{ie\uparrow} (d^n/d^{n-1}) \) well below the bottom of the conduction band. The notation \( (d^n/d^{n-1}) \), commonly accepted in the spectroscopy of deep d-states in semiconductors [12,13,21,27], means that the occupation of the level \( E_{ie\uparrow} \) corresponds to a change of the atomic configuration from \( d^{n-1} \) to \( d^n \) due to a transfer of a host spin-up electron to an e-state of the impurity 3d shell. The levels \( E_{ie\downarrow} \) are more shallow than \( E_{ie\uparrow} \) in accordance with the Hund rule, so that \( E_{\downarrow} - E_{ie\uparrow} \gg E_{\downarrow} - E_{ie\downarrow} \). Filling these levels begins when the 3d-shell is more than half-filled \( (n > 5 \), the elements from Fe to Ni). In this case both the \( E_{ie\uparrow} \) and \( E_{ie\downarrow} \) levels are deep below the bottom of the conduction band, and the resonance scattering is weak in accordance with Eq. (22).

As a result, one can expect that the effect of the resonance scattering will be strong for light elements (Ti, V, Cr, Mn), and resonance interaction splits the \( m = 0 \) states predominantly from the down-spin Landau subband, whereas the potential scattering is spin-independent. One can estimate the resulting spin splitting of the lowest impurity Landau levels, \( \Delta_{bs} \), from Eq. (24):

\[
\Delta_{bs} = \frac{|V_{eb}|^2}{\Delta_{\uparrow} \Delta_{\downarrow}} \Delta_{es},
\]

where \( \Delta_{\uparrow} \) and \( \Delta_{\downarrow} \) are the spin splitting in the conduction band and \( \Delta_{es} \) is the spin parameter of the host material.
where $\Delta_{e\downarrow} = \varepsilon_{e\downarrow} - \varepsilon_{e\uparrow}$ is the exchange splitting of the impurity d-levels, $\Delta_e = E_b - \varepsilon_{e\sigma}$. The same kind of spin splitting exists for the impurity levels belonging to higher Landau bands. Fig. 3a illustrates the spin polarization of Landau states in this case.

Hund rule is known to be violated for V impurity in some III-V host crystals. Vanadium creates $e\sigma$-levels in the upper part of the semiconductor energy gap for both spin projections. There are numerous experimental [15] and theoretical [16] arguments in favor of the "anti-Hund" low-spin states $V^0(e_{i\uparrow}e_{\downarrow})$ and $V^- (e_{i\uparrow}^2e_{\downarrow})$ ions. Therefore, the resonance scattering is strong for both Landau subbands and, moreover, the levels $\varepsilon_{e\downarrow}$ and $E_b$ are nearly degenerate (Fig. 3b). In the case of a Cr ion the level $\varepsilon_{e\downarrow}$ is in resonance with the states above the bottom of the conduction band in bulk GaAs, so the inequality $E_b < \varepsilon_{e\downarrow}$ is valid (Fig. 3c). Then the spin splittings of the Landau bound states and the impurity $d$ states have the opposite signs (see next section). When calculating $\Delta_{bs}$ in this case, one should use full Eq. (20) instead of approximate Eq. (22).

Especially interesting is the case of Mn. Substitutional Mn ions retain half filled d shell (Mn(d$^5$)) with the maximal spin $S = 5/2$ according to the Hund rule) both in III-V and in II-VI compounds. The corresponding levels $E_\gamma$ (d$^5$/d$^4$) lie deep in the valence band (see, e.g. [19]). This means that the resonance scattering for spin up electrons is extremely weak. The resonance level $E_{e\downarrow}$ corresponds to the empty state Mn(d$^6$/d$^5$). This state was never observed directly, but indirect data for some III-V [20] and II-VI compounds [21] indicate that such a level may exist within the conduction band not far from its bottom. This means that Mn impurity corresponds to the extreme limit of the case (c) in Fig. 3. It should be mentioned that practically the same mechanism of the magnetic coupling between TM ion and conduction electrons via hybridization $V_{\mu\lambda}$ [9] was considered for the specific case of (Cd,Mn)Te/(Cd,Mn,Mg)Te heterostructures in Ref. [22]. Here the case of zero magnetic field was considered, and $\lambda$ included confined electrons near the edges of the valence and conduction bands. It was shown in this paper that the "kinetic" antiferromagnetic exchange $\sim |V_{\gamma\mu}\lambda|^2/(E_\lambda - E_\gamma)$ even in the case of a very deep $d$-level is strong enough to compensate essential part of the direct ferromagnetic exchange between the localized impurity spin and the band carriers.

The spin-split Landau levels can be occupied by the electron-hole pairs, and one can treat such pairs as the bound magnetic excitons which appear on the background of conventional spin waves and magnetoplasmons in 2DES. The theory of magnetic excitations bound with 3$d$ impurities based on the methods of conventional theory of magnetic excitations in 2DES [13,14] will be published elsewhere.

\[ \begin{array}{c|c|c|c}
 n = 0 & E_{b0\uparrow} & E_{i\sigma\downarrow} & E_{i\sigma\uparrow} \\
 \hline
 1 & E_{b1\uparrow} & E_{i\sigma\downarrow} & E_{i\sigma\uparrow} \\
 \hline
 2 & E_{b2\uparrow} & E_{i\sigma\downarrow} & E_{i\sigma\uparrow} \\
 \end{array} \]

FIG. 3. Energy levels for the bound states: (a) weak scattering limit for both, $\uparrow$ and $\downarrow$ states; (b) strong resonance scattering for $\downarrow$ states; (c) the resonance level for the $\downarrow$ states above the lowest Landau levels.

**IV. IMPURITY $g$ FACTOR**

During the last three decades the oscillatory enhancement of the $g$ factor of delocalized electrons in 2DES was studied both experimentally [23,24] and theoretically [24,25]. The oscillatory behavior of the $g$ factor in a 2DES is explained by a variation of the many-body Coulomb and exchange renormalizations of the Zeeman splitting as a function of the occupation of Landau subbands.

In this section we consider the behavior of the electronic $g$ factor due to the impurity scattering. As was shown in the previous section, the spin splitting of local states with $m = 0$ in Landau subband may exists even in the absence of an external magnetic field due to the spin selectivity of the resonance impurity scattering. The mixed nature of
for the spin-down states, so that sin $\theta$ is localized when the magnetic length decreases. Therefore, in the weak scattering limit both contributions to the hybridization matrix element (21) increases with the growing magnetic field since the wavefunction scattering channel. The second contribution to the enhancement mechanism stems from the orbital effect: the $d$ admixture of the polarization of the approximation (22), we find that the inequality sin $\theta$ may vary in a wide range.

Three examples of spin splitting illustrated by Fig. 3 show the variety of possible modifications of the $g$ factor as well. Let us start with considering the Zeeman splitting of the electrons in the lowest localized Landau state (weak scattering limit of Fig. 3a). In this case the deep d-levels $E_{\ell \uparrow\downarrow}$ with both spin projections are occupied and the effective $g$ factor of the impurity is predetermined by the Zeeman shift of the antibonding levels $E_{e\uparrow}$. It may be calculated by means of the simplified Eq. (22) or its corollary (23). We define the effective $g$ factor in the usual way,

$$
\langle \hat{\psi}_i | H_z | \hat{\psi}_i \rangle = \pm \frac{1}{2} \mu_0 B \parallel g_{eff},
$$

where $\hat{\psi}_i$ is the eigenvector with the components $\psi_{i\sigma}^{(b,a)}$ which correspond to the solutions (22) of the effective two-level problem.

$$
\begin{align*}
\psi_{i\sigma}^b &= \cos \theta_\sigma \psi_{ie\sigma} + \sin \theta_\sigma \psi_{i\sigma b} \\
\psi_{i\sigma}^a &= - \cos \theta_\sigma \psi_{i\sigma b} + \sin \theta_\sigma \psi_{i\sigma e}
\end{align*}
$$

with the mixing coefficient given by

$$
\tan 2\theta_\sigma = \frac{2V_{eb}}{\Delta_\sigma}.
$$

$H_z$ is the Zeeman Hamiltonian

$$
H_z = \mu_0 (K\mathbf{L} + g_0 \mathbf{S}) \mathbf{B},
$$

$\mathbf{S}$ and $\mathbf{L}$ are the spin and orbital angular moments, $K$ is the covalency reduction factor. In our specific case of the bound s-states the orbital contribution is absent. Extracting from (24) the antibonding component $\psi_{i\sigma}^e$, we find, in the limit

$$
\sin \theta_\sigma \approx \frac{V_{eb}}{\Delta_\sigma} \ll 1
$$

and in the linear approximation in the magnetic field, that

$$
\delta g = g_{eff} - g_b \approx - \frac{V_{eb}^2}{\Delta_\uparrow \Delta_\downarrow} \left[ \bar{g} \left( 1 + \frac{\Delta_\uparrow^2}{2\Delta_\uparrow \Delta_\downarrow} \right) + \Delta_{es} L (|V_{eb}|^2) \right].
$$

Here $\bar{g} = g_b - g_d$ and $g_b,d$ are the $g$ factors of the Landau electron and the $d^n$ ion, respectively,

$$
g_d = g_s + g_L + \Delta g,
$$

g_s and $g_L$ are the contributions to the $g$-factor due to the projections of the spin and orbital moments on the total angular moment. $\Delta g$ contains contributions due to the spin-orbit interaction, electron-phonon interaction, etc. These corrections are specific for a given ion in a given host semiconductor (see, e.g., [13]). Both the value and the sign of $\bar{g}$ may vary in a wide range. $L(A) = A^{-1} \partial A / \partial h$ is the logarithmic derivative, $h = \mu_0 B$.

It is seen from Eq. (23) that there are two contributions into the enhancement of the $g$ factor. The first one is an admixture of the polarization of the $d$ shell of the TM impurity to the spin splitting of Landau states via the resonance scattering channel. The second contribution to the enhancement mechanism stems from the orbital effect: the hybridization matrix element (21) increases with the growing magnetic field since the wavefunction $\psi_b(\xi; E_{ba})$ becomes stronger localized when the magnetic length decreases. Therefore, in the weak scattering limit both contributions to the effective $g$ factor are positive provided $\bar{g} < 0$, and in this case we deal with the enhancement (see below).

The renormalization of the $g$ factor of the bound Landau electrons is more pronounced in the case when the Landau level $E_{b\uparrow}$ and the impurity level $\varepsilon_{\mu\downarrow}$ are nearly degenerate (Fig. 3b). Then, confining ourselves with the two-level approximation (22), we find that the inequality $\sin \theta_\uparrow \ll 1$ is valid for the spin-up states, whereas the mixing is strong for the spin-down states, so that $\sin \theta_\downarrow \approx 1/\sqrt{2}$. Neglecting the orbital contribution we find that

$$
\delta g_b = \frac{\bar{g}}{4} \left( 1 - \frac{|\Delta_\downarrow|^2}{2|V_{eb}|^2} \right).
$$

9
Here $-\bar{g}/4$ makes the principal contribution, and the two other terms describe hybridization corrections for the spin-down and -up states.

As expected, the sign and the magnitude of the $g$ factor renormalization is predetermined by the difference $\bar{g}$. The $g$ factor of the Landau electrons in the 2DES formed in GaAs is small $g_0 \ll g_0$ where $g_0 = 2.003$. On the other hand, the $g$ factor of 3d-ions varies from one element to another. It also depends on the charge state of the given impurity and may be influenced by local defects in the host crystal [13,27]. However, nearly in all states its value is close to $g_0$. On the other hand, the $g$ factor of 3d-ions varies from one element to another. It also depends on the charge state of the given impurity and may be influenced by local defects in the host crystal [13,27]. However, nearly in all states its value is close to $g_0$. In particular, $gd = 1.957$ for $V^{3+}$, $gd = 1.974$ for $Cr^{3+}$ in bulk GaAs. The value of $gd \approx 1.60$ was reported for $V^{2+}$ [28], but this reduction is due to the orthorhombic distortion of crystalline environment in this specific sample. So we can assume in our estimates that $\bar{g} \sim -1$ in the cases of our interest, and the $g$ factor renormalization is, in fact, an enhancement.

To estimate the corrections to the maximum value of $\delta g_b = -\bar{g}/4$ given by Eq. (29) one should notice that all three gaps $\Delta_1, \Delta_1, \Delta_{es}$ are of the same order in the range 0.5 to 1 eV in the weak scattering case (27), and the hybridization parameter normally does not exceed 0.1 to 0.2 eV.

The last term in the brackets of Eq. (28) can be evaluated by means of Eq. (15) which is valid in the limit $\xi \gg 1$ (the magnetic length is essentially larger than the radius of the d-wave function). A decrease of of the relative weight of the Bloch tail of the s-type wavefunction $\psi_b$ implies a corresponding growth of its "core" part, so that the resulting increase of the logarithmic derivative $L(|\psi_{eb}|^2)$ can be estimated as a small effect of the order of $(l_d/l_b)^2 \ll 1$, where $l_d \sim a_b$ is the radius of the d-part of the impurity wave function (5). Thus, the orbital contribution to the Zeeman splitting is small in comparison with the paramagnetic one. We conclude that even in this weak scattering limit the magnitude of enhancement can be estimated as an effect $\sim (V_{eb}/\Delta_\sigma)^2$ which is up to 10% above $g_0$.

In case of partially occupied Landau bands, an experimental observation of a contribution of the b-levels with $m = 0$, split off the Landau bands $E_n \neq 0$, on the background of other states filling the gaps between Landau levels (Fig. 2) may be not an easy task. At small TM impurity concentrations the strongest observable effect involving Zeeman splitting is a variation of the impurity d-shell occupation in a quantizing magnetic field. The hybrid structure of the impurity states can be detected when studying the d-electron $g$ factor, e.g., by methods of ESR spectroscopy, provided the impurity configuration is $e_1b^2n$, i.e., the level $E_{i1}$ is empty in the zero magnetic field. Noticeable effects are expected when $E_{i1}$ is slightly above the Fermi level $\varepsilon_F$ of the conduction electrons in the zero magnetic field. (Fig. 4).

---

**FIG. 4.** Relative positions of bound Landau states $E_{2m+1}$ (thick solid lines), free Landau levels $E_n$ (thin dashed lines), resonant level $\varepsilon_{ie}$ (thick dashed line) and the Fermi level $\varepsilon_F$ in the zero magnetic field (thin line) and in a quantizing magnetic field (thick dotted line). See text for further explanations.

The dotted saw-tooth-like curve in this figure shows the oscillations of the Fermi level $\varepsilon_F(B)$ that reflect the jumps $\delta_n$ from the filled Landau level $E_n$ to the next Landau level $E_{n+1}$ at $B = B_n$. These jumps $\delta_n = h^2/2m_l^2B_n$ are smoothed, since the inter-level windows are filled with impurity states of various origin (see Fig. 2). Since the diamagnetic shift of the Landau levels with an increasing magnetic field becomes essentially bigger than the Zeeman splitting.
(\(\hbar^2/2m^*l_0^2 \gg g\mu_BB\)), the latter effect can be neglected in this evolution of the spectrum. Then with increasing field \(B\), the impurity e-level will cross all Landau levels, and eventually, at a high enough magnetic field, it will be squeezed out into the energy gap below the first Landau level. If the difference \(E_{iL} - \varepsilon_F < \delta_n\), then the occupation of the d-shell changes from \(e^i b^{2n}\) to \(e^i b^{2n}\) within some intervals \(B_1' \div B_1\) and \(B_2' \div B_2\) of the magnetic field (hatched domains in Fig.4), and the ESR signal should disappear in these regions. Small dips in \(g_d\) due to an admixture of the b-states may be also observed near the points \(B_3, B_4, \) etc.

Recent achievements in fabricating heterostructures with large manganese contents, e.g., (In, Mn)As/(Al, Ga)Sb, (Cd, Mn)Te/(Cd, Zn, Mg)Te [see, e.g., [9]] open a new possibility of tuning the electron position of the resonance level \(E\), when the potential considered in [7,8], can be summarized as follows: (i) the appearance of the charged bound states. The sharpness of this effect may be also observed in TM dimers at low temperatures and the potential dependence of the electron occupation in d-shell. It is worth noting that the reduction of the \(g\) factor will change in accordance with equations (28) and (29) each time when the level \(\varepsilon_{ieL}\) crosses a bound Landau level \(\varepsilon_{bnL}\). Probably, the minor oscillations of the \(g\)-factor, observed on the background of the strong \(g\)-factor change due to the above concentration effects in magneto-optical spectra of (Cd, Mn)Te/(Cd, Mg)Te [10] heterostructures, can be explained by the mechanism proposed in this section. These oscillations will be a subject of our future investigation.

V. CONCLUSIONS

This paper demonstrates that the Landau quantization makes dramatic changes in the structure of localized states in semiconductors doped by magnetic impurities. We concentrate here on the appearance of bound Landau states near the bottom of the conduction band. It is found that both orbital and spin parts of the impurity scattering potential are significant. We consider TM ions substituting cations in III-V semiconductors and have found that both short-range potential and resonance components of impurity scattering influence mainly the states with the zero orbital momentum \(m = 0\).

New features introduced by the resonance component of the scattering potential, as compared to the short range potential considered in [11], can be summarized as follows: (i) the sign of the scattering potential depends on the position of the resonance level \(E_{ie}\): the resonance scattering partially cancels the short-range potential scattering, when \(E_{ie} - E_b < 0\), and enhances it, when \(E_{ie} - E_b > 0\); (ii) the resonance scattering plays a decisive part in appearance of the charged bound states.

The role of spin effects is more profound: the fact that the spin state of a TM ion is determined by the interatomic Coulomb and exchange interaction, makes the resonance scattering spin selective. Its influence on the Landau states also depends on the spin state of the Landau orbitals. The most striking manifestation of this spin selectivity is a possibility of a significant enhancement of the \(g\) factor of the localized Landau states. This enhancement may be noticed in magneto-optical measurements.

The same resonance scattering results also in noticeable changes of the properties of the electronic states of TM impurities: (i) removal of the symmetry ban for hybridization between the de-states and s-states for the conduction band may result in a considerable increase of the crystal field splitting \(\Delta_{CF}\); (ii) reduction of the \(g\) factor of the d-electrons is dual to that of the corresponding Landau states, so that an experimental possibility arises to study properties of bound states in Landau bands by measuring the \(g\) factor of the impurity \(d\)-shell. It is worth noting that the reduction of the \(g\) factor may be responsible for an enhancement of the nuclear spin relaxation, because it partially compensates the difference in the energy scales of nuclear and electronic subsystems.

The modification of the one-electron spectrum of a 2DES by the impurity scattering should also be accompanied by changes in the spectrum of spin excitons, magnetoplasmons and other collective excitations in strongly quantized electron gas. These effects will be described in forthcoming publications.

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