

Electron g factor in one- and zero-dimensional semiconductor nanostructures

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(Received 20 July 1998)

We investigate theoretically the Zeeman effect on the lowest confined electron in quantum wires and quantum dots. A general relation is established between the symmetry of a low-dimensional system and properties of the electron g factor tensor, $g_{\alpha\beta}$. The powerful method used earlier to calculate the transverse g factor in quantum wells is extended to one-dimensional (1D) and 0D zinc-blende-based nanostructures and analytical expressions are derived in the frame of Kane's model for the g factors in quantum wells, cylindrical wires, and spherical dots. The role of dimensionality is illustrated on two particular heteropairs, GaAs/Al_xGa_{1-x}As and Ga_{1-x}In_xAs/InP. The efficiency of the developed theoretical concept is demonstrated by calculating the three principal values of the g factor tensor in rectangular quantum wires in dependence on the wire width to establish also the connection with the 2D case. [S0163-1829(98)01547-1]

I. INTRODUCTION

In bulk semiconductors with zinc-blende lattice the effective electron Landé factor depends strongly on the fundamental energy gap and the spin-orbit splitting of the topmost valence band. It varies in a wide range from a large negative value in narrow-gap semiconductors (e.g., about -50 in InSb) to positive values $g \leq 2$ in wide-gap materials. This behavior is accounted for by the well-known Roth equation derived in second-order $\mathbf{k} \cdot \mathbf{p}$ perturbation theory.¹⁻³ The $\mathbf{k} \cdot \mathbf{p}$ theory was extended from bulk materials to zinc-blende based heterostructures, quantum wells (QW's), and superlattices, including calculations of the conduction electron g factor as a function of the layer widths.⁴ The theory predicted a large confinement-induced anisotropy of the Zeeman effect: the difference between the longitudinal (g_{\parallel}) and transverse (g_{\perp}) components of the g -factor tensor (obtained for magnetic fields $\mathbf{B} \parallel$ or \perp , respectively, to the growth axis z) was found in the same order of magnitude as these values themselves. The Zeeman splitting of electron spin states in biased QW structures has been calculated in Ref. 5.

Detailed measurements performed on the transverse electron g factor, $g_{\perp}(L_z)$, as a function of the well width L_z for GaAs/Al_{0.3}Ga_{0.7}As QW structures⁶⁻⁸ showed the sign change of g_{\perp} at $L_z \approx 65$ Å. Moreover, a giant difference between g_{\parallel} and g_{\perp} has been observed on A_3B_5 and A_2B_6 based heterostructures, namely in GaAs/Al_xGa_{1-x}As, GaAs/AlAs, Ga_{1-x}In_xAs/InP, and CdTe/CdMgTe, under optical orientation of free carriers in tilted magnetic fields,⁹⁻¹¹ in optically detected magnetic resonance (ODMR) experiments,^{12,13} by using the quantum beat technique,¹⁴ and in resonant spin-flip Raman scattering.¹⁵⁻¹⁷ First measurements of the electron and hole g factors for InP/In_xGa_{1-x}P quantum dots as reported more recently¹⁸ indicate the interest in extending the theoretical concepts of the electron g factor to systems of lower dimension.

In the present paper we develop a theory of the Zeeman effect for electrons in quasi-one- and quasi-zero-dimensional

systems, i.e., in quantum wires (QWR's) and quantum dots (QD's). In the next two sections we present the general theoretical considerations and derive an equation for the tensor components of the electron g factor in the Kane model. The results on cylindrical QWR's and spherical QD's are given in Sec. IV. The g -factor tensor in a rectangular QWR is calculated in Sec. V.

II. GENERAL THEORY

For a pair of Kramers-conjugate states, the Zeeman contribution to the electron effective Hamiltonian is written as

$$\frac{1}{2} \mu_0 \sigma_{\alpha} g_{\alpha\beta} B_{\beta},$$

where σ_{α} ($\alpha = x, y, z$) are the Pauli matrices, \mathbf{B} is the magnetic field, μ_0 is the Bohr magneton and, for a low-symmetry system, the real tensor $g_{\alpha\beta}$ is characterized by nine linearly independent components.⁵

In general, the effective g factor results from second-order perturbation theory¹ and, thus, is expressed as a sum over intermediate states. For an electron in the lowest s -antibonding conduction band of Γ_{6c} symmetry in a zinc-blende semiconductor with T_d symmetry, one has $g_{\alpha\beta} = g \delta_{\alpha\beta}$ with

$$g = g_0 + \frac{1}{m_0 n \neq \Gamma_{6c}} \sum \frac{|P_{c,1/2;n}^+|^2 - |P_{c,1/2;n}^-|^2}{E_{\Gamma_{6c}}^0 - E_n^0}, \quad (1)$$

where m_0 and $g_0 \approx 2$ are the free-electron mass and Landé factor, the index n runs over higher and lower bands, E_n^0 is the electron energy at the Γ point, $P_{c,s;n}^{\pm} = \langle c\Gamma_{6c}, s | P_x \pm iP_y | n \rangle$, the spin index $s = \pm 1/2$, and \mathbf{P} is the momentum operator. It should be noted that Eq. (1) can be as well derived straightforwardly as a first-order correction due to magnetic field-induced perturbation⁵

$$\delta H = \frac{e}{c} \mathbf{A} \cdot \mathbf{V}$$

to the electron Hamiltonian. Here \mathbf{V} is the velocity operator, $-e$ is the electron charge, and $\mathbf{A}(\mathbf{r})$ is the vector-potential, which for a homogeneous magnetic field is a linear function of the radius vector \mathbf{r} . In order to derive the second term on the right-hand side of Eq. (1), one can rewrite the matrix element $\langle c\Gamma_{6,1/2} | \mathbf{A} \cdot \mathbf{V} | c\Gamma_{6,1/2} \rangle$ as a product of the matrix elements $\langle c\Gamma_{6,1/2} | \mathbf{A} | n \rangle$ and $\langle n | \mathbf{V} | c\Gamma_{6,1/2} \rangle$ summed up over all states n and use the equation (see, e.g., Refs. 19 and 20)

$$\langle n\mathbf{k} | \mathbf{r} | n'\mathbf{k}' \rangle = i\delta_{nn'} \frac{\partial}{\partial \mathbf{k}} \delta_{\mathbf{k}\mathbf{k}'} + \Omega_{nn'}(\mathbf{k}) \delta_{\mathbf{k}\mathbf{k}'}, \quad (2)$$

$$\Omega_{nn'}(\mathbf{k}) = i \int d\mathbf{r} u_{nk}^* \frac{\partial}{\partial \mathbf{k}} u_{n'k}(\mathbf{r}),$$

for the matrix element of the radius-vector taken between the Bloch states $e^{i\mathbf{k}\cdot\mathbf{r}} u_{nk}(\mathbf{r})$ and $e^{i\mathbf{k}'\cdot\mathbf{r}} u_{n'k'}(\mathbf{r})$. At the final stage of derivation one can use the identity $\langle n\mathbf{k} | \mathbf{P} | n'\mathbf{k}' \rangle = 0$ for degenerate states and the conventional relation between the interband matrix elements of coordinate and velocity. It follows then that for the Bloch states in bulk semiconductors the approach based on the first-order correction δH gives no advantages as compared with the second-order $\mathbf{k}\cdot\mathbf{p}$ theory and in both approaches one has eventually to perform the summation in Eq. (1). In typical zinc-blende semiconductors the main contribution to g comes from the upper valence bands Γ_{8v}, Γ_{7v} and the electron g factor is given by¹⁻³

$$g = g_0 - \frac{4}{3} \frac{m_0 P^2}{\hbar^2} \frac{\Delta}{E_g(E_g + \Delta)}, \quad (3)$$

where E_g is the band gap, Δ is the spin-orbit splitting of the valence band, and $P = i(\hbar/m_0) \langle S | P_z | Z \rangle$ is the Kane momentum matrix element formed between the s -antibonding conduction and p -bonding valence-band states.

Of course an equation similar to Eq. (1) can be used for heterostructures, particularly for QW structures and superlattices.⁴ In this case, however, the index n runs not only over the different bands but also over subbands or minibands formed as a result of the quantum confinement with the consequence that the convergence is as a rule rather poor, the calculation procedure turns out to be cumbersome, and actually excludes possibilities for the analysis of simple limiting cases.

On the other hand, low-dimensional structures allow an efficient alternative approach based on the spatial confinement of the electron wave function which has been applied recently to calculate the transverse g factor in QW's.⁵ Indeed, if the wave function is localized in the direction ζ , the diagonal matrix element of the coordinate ζ is no longer a functional like Eq. (2) and the matrix element of δH for $\mathbf{B} \perp \zeta$ can be calculated avoiding its transformation into the sum in Eq. (1). Thus, for the conduction-electron ground state $e1$ in a QD, the Zeeman Hamiltonian is written in the alternative approach as

$$\frac{1}{2} \mu_0 \sigma_{\alpha,ss'} g_{\alpha\beta} B_\beta = \frac{1}{2} g_0 \mu_0 \eta_{\alpha,ss'} B_\alpha + \langle e1, s | \delta H | e1, s' \rangle, \quad (4)$$

where $s, s' = \pm 1/2$ and $\eta_{\alpha,ss'} = \langle e1, s | \sigma_\alpha | e1, s' \rangle$. The difference between $\eta_{\alpha,ss'}$ and $\sigma_{\alpha,ss'}$ arises from an admixture in the state $|e1, s\rangle$ of the opposite spin $-s$. Numerical estimates show that this difference is very small in all particular cases considered below and hereafter it is neglected. Equation (4) is applicable as well for the electron state at the $e1$ -subband bottom in a QWR provided that the vector potential gauge is chosen in such a way that $\mathbf{A}(\mathbf{r})$ depends on a coordinate perpendicular to the wire principal axis and the diamagnetic contribution

$$\frac{e}{c} \langle A_z \rangle \langle e1, s | V_z | e1, s' \rangle$$

is excluded from the matrix element $\langle e1, s | \delta H | e1, s' \rangle$. Note, that the average $\langle A_z \rangle \equiv \langle e1, s | A_z | e1, s \rangle$ is independent of the spin s and the matrix elements $\langle e1, s | V_z | e1, s' \rangle$ determine the linear-in- k_z terms in the electron energy dispersion in QWR's with low-symmetry cross sections.

In the multiband model, the effective Hamiltonian $H(\mathbf{k})$ is a matrix with the components $H_{nn'}(\mathbf{k}) = E_n^0 \delta_{nn'} + (\hbar/m_0) \mathbf{k} \cdot \mathbf{P}_{nn'} + (\hbar^2 k^2 / 2m_0) \delta_{nn'}$. If one neglects the small contribution arising from the third term, then the velocity operator $\mathbf{V} = \hbar^{-1} \partial H(\mathbf{k}) / \partial \mathbf{k}$ is represented by a matrix with \mathbf{k} -independent components. This means that the magnetic-field-induced correction δH is a matrix with components linearly dependent on ζ . Therefore, in order to calculate the components $g_{\alpha\beta}$, it suffices to find, first, the electronic states $|e1, s\rangle = \sum_n \varphi_n(\mathbf{r}) |n\rangle$ at zero magnetic field and, second, the matrix elements $\int d\mathbf{r} \varphi_n^*(\mathbf{r}) \zeta \varphi_{n'}(\mathbf{r})$, where the integration is performed separately over every structure volume bounded by interfaces. We would like to stress that here n is the index enumerating only the electronic bands in the corresponding bulk compositional semiconductors but not the quantum-confined states. In the following section, we derive an equation for the matrix element $\langle e1, s | \delta H | e1, s' \rangle$ in Eq. (4) by using the Kane model.

III. ELECTRON g FACTOR IN THE KANE MODEL

The Kane model explicitly takes into consideration the $\mathbf{k}\cdot\mathbf{p}$ mixing between the lowest conduction band Γ_{6c} and the highest valence band Γ_{8v}, Γ_{7v} states and ignores coupling with other bands. The multiband $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian $H(\mathbf{k})$ reduces to an 8×8 matrix. Following Suris²¹ we present the electron wave function in the form

$$\Psi = uS + v_x X + v_y Y + v_z Z,$$

where $u(\mathbf{r})$ and $\mathbf{v}(\mathbf{r})$ are spinor envelope functions. In terms of u and \mathbf{v} , the Schrödinger equation is conveniently written as follows:

$$Eu = -iP\hat{\mathbf{k}} \cdot \mathbf{v} \quad (5)$$

$$\left(E + E_g + \frac{\Delta}{3} \right) \mathbf{v} = iP\hat{\mathbf{k}}u + i\frac{\Delta}{3} \boldsymbol{\sigma} \times \mathbf{v}.$$

Here E is the electron energy with respect to the bottom of the conduction band Γ_{6c} , $\hat{\mathbf{k}} = -i\nabla$, and the parameters E_g , Δ , and P are introduced in Eq. (3). By using the second equation (5) one can express the vector spinor \mathbf{v} via the gradient ∇u as

$$P\mathbf{v} = \frac{\hbar^2}{2m_c(E)}\nabla u - i\frac{\hbar^2}{4m_0}[g(E) - g_0](\boldsymbol{\sigma} \times \nabla)u, \quad (6)$$

where

$$\frac{1}{m_c(E)} = \frac{2}{3}\frac{P^2}{\hbar^2}\left(\frac{2}{E_g + E} + \frac{1}{E_g + E + \Delta}\right), \quad (7)$$

$$g(E) = g_0 - \frac{4}{3}\frac{m_0 P^2}{\hbar^2}\frac{\Delta}{(E_g + E)(E_g + E + \Delta)}.$$

Substituting Eq. (6) into the first Eq. (5) we naturally come to a second-order differential equation for the conduction-band envelope,

$$\frac{\hbar^2 \hat{\mathbf{k}}^2}{2m_c(E)}u = Eu. \quad (8)$$

Boundary conditions are the continuity of the spinor $u(\mathbf{r})$ and of the normal component of the vector $P\mathbf{v}(\mathbf{r})$ at the interfaces. Note that $m_c^{-1}(0)$ and the difference $g(0) - g_0$ describe the valence-band $\mathbf{k} \cdot \mathbf{p}$ contributions to the inverse effective mass and the g factor at the bottom of the conduction band.

In the Kane model, the velocity operator $\hat{\mathbf{V}} = \hbar^{-1}\partial H(\mathbf{k})/\partial \mathbf{k}$ is an 8×8 matrix with \mathbf{k} -independent components. Using the explicit form for this matrix, we obtain

$$\langle e1, s | \delta H | e1, s' \rangle = i\frac{e}{c\hbar} \int P[(\mathbf{A} \cdot \mathbf{v}_s^+)u_{s'} - u_s^+(\mathbf{A} \cdot \mathbf{v}_{s'})]d\mathbf{r}. \quad (9)$$

One can present the spinor wave function $u(\mathbf{r})$ in the general form as

$$u_s(\mathbf{r}) = [f(\mathbf{r}) + i\sigma_\alpha h_\alpha(\mathbf{r})]c_s, \quad (10)$$

where $f(\mathbf{r}), h_\alpha(\mathbf{r})$ are real functions and c_s ($s = \pm 1/2$) are the spin-up and spin-down states, respectively. Symmetry of a quantum heterosystem imposes restrictions on the coordinate dependence of these functions. In particular, for the ground electron state $e1$ in a QD of the point symmetry D_{2h} (the symmetry of a rectangular box or an ellipsoid), one has

$$f(\mathbf{r}) = f(x^2, y^2, z^2), \quad h_x(\mathbf{r}) = yz M_x(x^2, y^2, z^2),$$

$$h_y(\mathbf{r}) = zx M_y(x^2, y^2, z^2), \quad h_z(\mathbf{r}) = xy M_z(x^2, y^2, z^2),$$

where f and M_α are arbitrary functions of x^2 , y^2 , and z^2 . For the conduction-electron state $e1$ at the subband bottom $k_z = 0$ in a QWR with rectangular cross section, the envelopes u, \mathbf{v} are independent of z , where z is the wire principal axis, and, hence,

$$h_z(\mathbf{r}) = xy M_z(x^2, y^2), \quad h_x(\mathbf{r}) \equiv h_y(\mathbf{r}) \equiv 0. \quad (11)$$

For QWR's with a cross section in the form of a regular N -sided polygon, $h_z(\mathbf{r}) = \text{Im}(x + iy)^N M_z(x, y)$, where $M_z(x, y)$ is an invariant of the point group D_{nh} . For example, for $n = 4$, i.e., in the case of a quadratic cross section,

$$h_z(\mathbf{r}) = xy(x - y)(x + y)F(x^2, y^2), \quad (12)$$

where $F(x^2, y^2) = F(y^2, x^2)$. In cylindrical wires, $f(\mathbf{r}) \equiv f(\sqrt{x^2 + y^2})$ while the three functions $h_\alpha(\mathbf{r})$ are identically equal to zero because there exist no polynomials $\Sigma_{l,m} C_{l,m} x^l y^m$ which transform as pseudovector components with respect to the group $D_{\infty h}$ operations. Due to similar reasons, in a spherical QD, $f(\mathbf{r}) \equiv f(\sqrt{x^2 + y^2 + z^2})$ and $h_\alpha(\mathbf{r}) \equiv 0$.

Substituting Eq. (10) into Eqs. (6) and (9), we finally arrive at the following main equations:

$$g_{\alpha\beta} = g_0 \delta_{\alpha\beta} + g_{\alpha\beta}^{(1)} + g_{\alpha\beta}^{(2)}, \quad (13)$$

$$g_{\alpha\beta}^{(1)} B_\beta = 4 \int d\mathbf{r} \{ f(\mathbf{A} \cdot \nabla) h_\alpha - h_\alpha (\mathbf{A} \cdot \nabla) f + H_\alpha^{(1)} \} \mu, \quad (14)$$

$$g_{\alpha\beta}^{(2)} B_\beta = 2 \int d\mathbf{r} \{ f(\mathbf{A} \times \nabla)_\alpha f - f[(\mathbf{A} \times \nabla) \times \mathbf{h}]_\alpha + H_\alpha^{(2)} \} G,$$

$$\mathbf{H}^{(1)} = \mathbf{h} \times (\mathbf{A} \nabla) \mathbf{h}, \quad H_\alpha^{(2)} = (\mathbf{A} \times \nabla) \mathbf{h} h_\alpha - \mathbf{h} (\mathbf{A} \times \nabla)_\alpha \mathbf{h},$$

governing the electron g -factor calculation in the approach outlined by Eq. (4). It is worth mentioning that for vanishing $h_\alpha(\mathbf{r})$ the contribution $g_{\alpha\beta}^{(1)}$ vanishes as well.

IV. SPHERICAL QD's AND CYLINDRICAL QWR's

For QD's of the spherical form, symmetry considerations and Eq. (6) allow us to write the spinors u and \mathbf{v} as

$$u_s(\mathbf{r}) = f(r)c_s, \quad (15)$$

$$P\mathbf{v}_s(\mathbf{r}) = \left[\frac{\hbar^2}{2m_c(E)} \frac{\mathbf{r}}{r} - i\frac{\hbar^2}{4m_0} [g(E) - g_0] \left(\boldsymbol{\sigma} \times \frac{\mathbf{r}}{r} \right) \right] \frac{df}{dr} c_s.$$

Due to the spherical symmetry of the function $f(r)$, the g -factor tensor is isotropic: $g_{\alpha\beta} = g \delta_{\alpha\beta}$. Since the normal to the spherical interface is directed along the radius vector \mathbf{r} , the normal component of $P\mathbf{v}_s$ is given by

$$\frac{\hbar^2}{2m_c(E)} \frac{df}{dr} c_s.$$

Therefore, the boundary conditions for a dot of the radius R reduce to the continuity of $f(r)$ and $m_c^{-1}(E)df/dr$ at $r = R$. In what follows, we denote the dot, wire, or well semiconductor material by A , the barrier material by B , and the mass $m_c(E)$ in the A or B materials by $m_A(E), m_B(E)$. For the ground-state solution of Eq. (8), one has $f(r) = Cr^{-1} \text{sink}r$, if $r \leq R$, and $C \text{sink}Rr^{-1} \exp[-\alpha(r - R)]$ for $r \geq R$, where

$$k = [2m_A(E)E/\hbar^2]^{1/2}, \quad \alpha = [2m_B(E)(\Delta E_c - E)/\hbar^2]^{1/2},$$

ΔE_c is the conduction-band offset at the A/B interface, and the coefficient C is fixed by the normalization condition

$$\int d\mathbf{r}(u^+u + \mathbf{v}^+ \cdot \mathbf{v}) = 1. \quad (16)$$

Note that taking into account the band offset, the mass $m_B(E)$ is defined as $m_c(E - \Delta E_c)$. It follows from Eqs. (13)–(15) that the electron g factor in a spherical QD can be presented by

$$g = g_0 - \frac{2}{3} \int dr r f \frac{df}{dr} [g(E) - g_0]. \quad (17)$$

Equation (15) is valid as well for a cylindrical QWR of the radius R provided the radius vector $\mathbf{r} = (x, y, z)$ and the modulus $r = |\mathbf{r}|$ are replaced by the two-dimensional vector $\boldsymbol{\rho} = (x, y)$ and $\rho = |\boldsymbol{\rho}|$. The $e1$ solution is given by $f(\rho) = CJ_0(k\rho)$ if $\rho \leq R$, and $DK_0(\kappa\rho)$ if $\rho \geq R$, where $J_0(x)$, $K_0(x)$ are the Bessel functions and $D = CJ_0(kR)/K_0(\kappa R)$. A nontrivial point is that the electron g factor in this case is also isotropic in spite of the uniaxial symmetry of the system. One can show straightforwardly that g_{xx} , g_{yy} , and g_{zz} coincide and are described by

$$g = g_0 - \int dx dy \rho f \frac{df}{d\rho} [g(E) - g_0]. \quad (18)$$

The isotropy is a consequence of the equation $u_s(\boldsymbol{\rho}) = f(\rho)c_s$, which means in particular that the three diagonal components $g_{\alpha\alpha}$ are proportional to the same two-dimensional integral with proportionality coefficients independent of the wire size. The coefficients must be equal because with increasing $R \rightarrow \infty$ the values of $g_{\alpha\alpha}$ tend to the same limit, i.e., to the electron g factor in the bulk semiconductor A .

After the partial integration, Eqs. (17) and (18) can be transformed into

$$g = g_0 + [g_A(E) - g_0]w_A + [g_B(E) - g_0]w_B + [g_B(E) - g_A(E)]V_{3-d}(R)f^2(R), \quad (19)$$

where V_n is a volume of the sphere in the n -dimensional space: $V_2 = \pi R^2$ and $V_3 = 4\pi R^3/3$, $g_A(E)$ and $g_B(E)$ are the values of $g(E)$ and $g(E - \Delta E_c)$ in the A and B materials, see Eq. (7), and w_A and w_B are the integrals $\int dr f^2(r)$ or $\int d\rho f^2(\rho)$ taken, respectively, over the A and B volumes. Note that the sum $w_A + w_B$ differs from unity because of the normalization (16). In the presentation by Eq. (19), the second and third terms can be attributed to volume contributions whereas the last term allows a natural interpretation as the interface contribution. An important point is that Eq. (19) describes as well the transverse g factor in a QW of the width $L_z = 2R$. In this case the dimensionality $d = 2$, the volume $V_{3-d} = 2R$, the spinor envelope $u_s(\mathbf{r}) = f(z)c_s$, $f = C \cos kz$ inside the QW, and $C \cos kR \exp[-\kappa(|z| - R)]$ outside the QW. For the longitudinal g factor in a QW, the proposed procedure cannot be applied in a straightforward manner because, if $\mathbf{B} \parallel z$, then for any gauge the vector potential \mathbf{A} depends on the in-plane coordinates and the matrix element of x or y taken between the quasi-two-dimensional electronic states is a functional. In Ref. 5, the component g_{\parallel} was found in a numerical calculation of the Landau levels and their spin

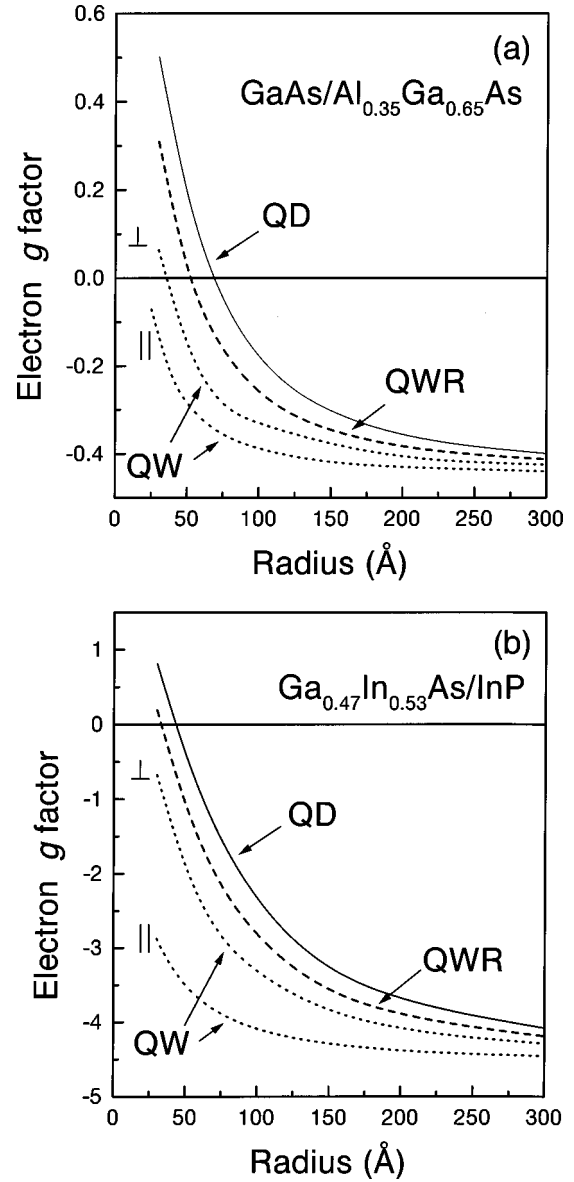


FIG. 1. The electron g factor calculated as a function of the radius R in spherical quantum dots (solid), cylindrical quantum wires (dashed), and quantum wells (dotted, $R = L_z/2$) for the heteropairs GaAs/Al_{0.35}Ga_{0.65}As (a) and Ga_{0.47}In_{0.53}As/InP (b).

splitting. In the next section we derive a compact equation for g_{\parallel} allowing a comparison with g_{\perp} given by Eq. (19) for $d = 2$.

Figure 1 shows the dependence of the electron g factor on the radius R in QD's and QWR's calculated for the isomorphic nanostructure GaAs/Al_xGa_{1-x}As and pseudomorphic structure Ga_{0.47}In_{0.53}As/InP. For comparison, in the same graph we present a variation of the longitudinal and transverse g factors in a QW. The parameters used in the calculation of the first heterosystem are as follows: $E_g = 1.52$ eV, $\Delta = 0.34$ eV, $2p_{cv}^2/m_0 = 28.9$ eV for bulk GaAs (here $p_{cv} = i\langle S|P_z|Z\rangle = m_0P/\hbar$); and $E_g = 1.94$ eV, $\Delta = 0.32$ eV, $2p_{cv}^2/m_0 = 26.7$ eV for bulk GaAs/Al_{0.35}Ga_{0.65}As, the band offset ratio $\Delta E_v : \Delta E_c = 2 : 3$. The contribution of remote bands is taken into account by adding the constant $\Delta g = -0.12$ to the Kane-model values of g . For the second heterosystem we used the following pa-

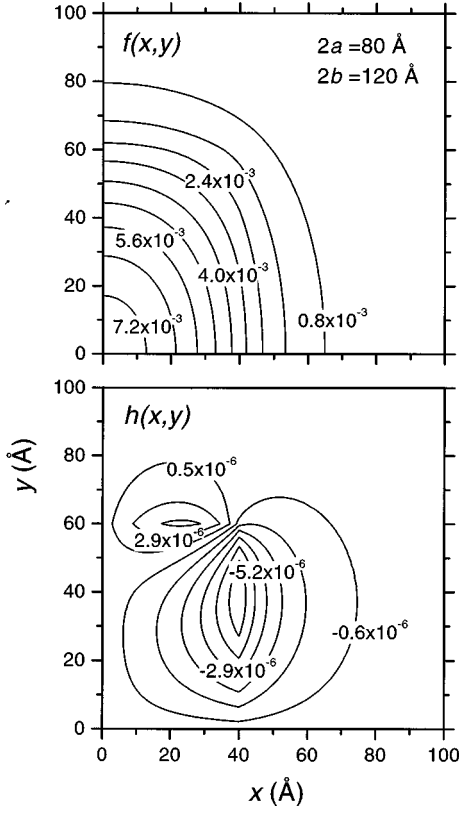


FIG. 2. Contour plots of the envelopes $f(x,y)$ and $h(x,y)$ for the electron lowest subband $e1$ (at the bottom $k_z=0$) in a $2a \times 2b$ rectangular GaAs/Al_xGa_{1-x}As QWR with $a=40$ Å and $b=60$ Å.

rameters: $E_g=0.813$ eV, $\Delta=0.356$ eV, $2p_{cv}^2/m_0=25.5$ eV for bulk Ga_{0.47}In_{0.53}As and $E_g=1.423$ eV, $\Delta=0.108$ eV, $2p_{cv}^2/m_0=20.4$ eV for InP, the valence-band offset $\Delta E_v=0.356$ eV, the contribution from remote bands $\Delta g=-0.13$. With increasing R the curves approach the bottom value of g in the bulk material A, in agreement with Eq. (19), where, for $R \rightarrow \infty$, w_A saturates to unity and values of w_B , E , and $V_{3-d}(R)f^2(R)$ tend to zero. The asymptotic behavior of g at large R is described by $g(R)=g_A(0)+\Delta g+(R_d/R)^2$ with the hierarchy $R_0 > R_1 > R_2^\perp > R_2^\parallel$, where R_2^\perp characterize the convergence of g_\perp and g_\parallel in QW's. In the opposite limit, $R \rightarrow 0$, the curves $g(R)$ tend to the g -factor value in the bulk barrier semiconductor, $g_B(0)+\Delta g=0.57$ in Al_{0.35}Ga_{0.65}As and 1.2 in InP. The relation $g^{\text{QD}} > g^{\text{QWR}} > g^{\text{QW}}$ can be understood taking into account that the reduction in dimensionality enhances the role of electron spatial confinement.

The estimation shows that the contribution of the term proportional to $f^2(R)$ in Eq. (19) is not relatively small, which excludes in general an approximate description of the dependence $g(R)$ in the simple form $g_A(E)w_A+g_B(E)w_B+\Delta g$.

V. RECTANGULAR QWR'S

Figure 1 demonstrates the main features of the effect of dimensionality on the electron g factor. Nevertheless, it is interesting to realize the proposed calculation scheme to a greater extent and consider less symmetrical structures where

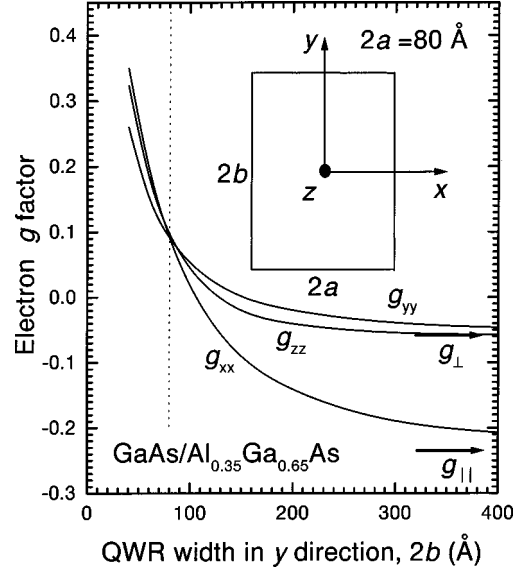


FIG. 3. The electron g factor components $g_{\alpha\alpha}$ ($\alpha=x,y,z$) in a GaAs/Al_xGa_{1-x}As rectangular QWR vs the length, $2b$, of one side. The other side, $2a$, is kept constant. The inset shows the orientation of the coordinate system. The arrows indicate values of the transverse and longitudinal g factors in the 80-Å-thick QW.

at least one of the functions $h_\alpha(\mathbf{r})$ in Eq. (10) is nonzero and where the tensor $g_{\alpha\beta}$ is characterized by three different diagonal components. This is the case for rectangular QWR's where $h_x(\boldsymbol{\rho})=h_y(\boldsymbol{\rho})=0$ but $h_z(\boldsymbol{\rho})\equiv h(\boldsymbol{\rho})\neq 0$. The continuous envelopes $f(\boldsymbol{\rho})$ and $h(\boldsymbol{\rho})$ satisfy Eq. (8); they are coupled at the interfaces by the continuity condition for the normal component of the spinor vector $P\mathbf{v}_s$ related to $\nabla\mathbf{u}_s$ by Eq. (6). This condition imposes the continuity requirement on the following two linear combinations of the derivatives ∇f and ∇h :

$$\begin{aligned} \mu \left(o_x \frac{\partial f}{\partial x} + o_y \frac{\partial f}{\partial y} \right) - \frac{G}{2} \left(o_x \frac{\partial h}{\partial y} - o_y \frac{\partial h}{\partial x} \right), \\ \mu \left(o_x \frac{\partial h}{\partial x} + o_y \frac{\partial h}{\partial y} \right) + \frac{G}{2} \left(o_x \frac{\partial f}{\partial y} - o_y \frac{\partial f}{\partial x} \right), \end{aligned} \quad (20)$$

where the axes x,y are directed along the rectangular sides, o_x, o_y are components of the two-dimensional unit vector \mathbf{o} normal to the A/B boundary, and $\mu=m_0/m_c(E)$, $G=g(E)-g_0$.

In order to find the ground-state solution $|e1,s\rangle$ of Eq. (8) in a wire of the cross section $2a \times 2b$, we applied the free relaxation technique described in Ref. 22. The envelopes $f(\boldsymbol{\rho})$ and $h(\boldsymbol{\rho})$ calculated for the GaAs/Al_{0.35}Ga_{0.65}As QWR 80 Å \times 120 Å are shown in Fig. 2 as contour maps. The origin of the coordinate system (x,y) is chosen in the wire center. Due to the rectangular symmetry it is enough to present the variation of f and h only in the quadrant $x,y > 0$. The function $f(x,y)$ has the maximum value $f_{\text{max}} \approx 7 \times 10^{-3}$ at the center and monotonously decreases with increasing radial distance ρ . In accordance with Eq. (11), the function $h(x,y)$ is zero if $x=0$ or $y=0$. It follows from Eq. (12) that for coinciding a and b this function should vanish also at the diagonal $x=y$ and have opposite signs at the points (x,y) and (y,x) . One can see in Fig. 2 areas of oppo-

site signs in the map of $h(x,y)$ in spite of a remarkable difference between a and b . As a result, in every quadrant the function $h(x,y)$ exhibits a maximum and a minimum. As compared with f_{\max} , the extremum values of $h(x,y)$ are smaller by three orders of magnitude.

The symmetry allows for the g -factor tensor, Eq. (13), to have only nonzero diagonal components. Because of the small values of h , we can ignore h^2 -like terms in the integrals of Eq. (14) and retain only f^2 - and fh -like terms. Taking into account that, for rectangular QWR's, $h_x = h_y = 0$ and $f, h_z \equiv h$ are z independent (z is parallel to the wire principal axis), Eqs. (13) and (14) are reduced into

$$\begin{aligned} g_{xx} &= g_0 - 2 \int dx dy y G \left(f \frac{\partial f}{\partial y} + f \frac{\partial h}{\partial x} \right), \\ g_{yy} &= g_0 - 2 \int dx dy x G \left(f \frac{\partial f}{\partial x} - f \frac{\partial h}{\partial y} \right), \\ g_{zz} &= g_0 - 2 \int dx dy x \left[G f \frac{\partial f}{\partial x} - 2\mu \left(f \frac{\partial h}{\partial y} - h \frac{\partial f}{\partial y} \right) \right] \\ &\equiv g_0 - 2 \int dx dy y \left[G f \frac{\partial f}{\partial y} + 2\mu \left(f \frac{\partial h}{\partial x} - h \frac{\partial f}{\partial x} \right) \right]. \end{aligned} \quad (21)$$

Figure 3 shows the dependence of g_{xx} , g_{yy} , and g_{zz} in GaAs/Al_{0.35}Ga_{0.65}As QWR's on one of the rectangular sizes while another size is kept constant and equal to $2a = 80 \text{ \AA}$.

With increasing b the components g_{yy} and g_{zz} converge on the electron transverse g factor in a QW of thickness 80 \AA and the component g_{xx} approaches the QW value of g_{\parallel} . In the square-shaped QWR, $b = a$, the two components g_{xx} and g_{yy} coincide as the symmetry predicts. Moreover, one can see from Fig. 3 that at the point $b = a$ the anisotropy $|g_{zz} - g_{xx}|$ is in fact quite small because, as it follows from Eq. (12), the function $h(x,y)$ vanishes at the four lines $x=0, y=0, y=x, y=-x$ and its values are too suppressed to produce a significant fh -like contribution.

In the Kane model defined by Eq. (5) we neglected the small free-electron-mass contribution $(\hbar^2 k^2 / 2m_0) \delta_{nn'}$ to the Hamiltonian $H_{nn'}(\mathbf{k})$ and the corresponding additional term $\delta H'_{nn'} = (e\hbar^2 / cm_0) \mathbf{A} \cdot \hat{\mathbf{k}} \delta_{nn'}$ in the magnetic-field-induced perturbation $\delta H_{nn'}$. In this connection we would like to note that the symmetry of a rectangular box or wire forbids non-zero values for the matrix elements $\langle e1, s | \delta H' | e1, s' \rangle$ because the product $A_\alpha \hat{k}_\alpha$ ($\alpha = x, y, z$) inverts its sign under reflection in the plane perpendicular to the axis α .

In the remaining part of this section we derive an equation for the electron longitudinal g factor in QW's by considering a rectangular QWR of the cross section $2a \times 2b$ and performing the asymptotic transition to infinite values of b . If $b \gg a$, then one can use an adiabatic approximation and write the envelope $f(x,y)$ inside the interval $(-b, b)$ and far enough from the ends $y = \pm b$ in the factorized form

$$f(x,y) = C \Phi(y) \begin{cases} \cos kx & \text{if } |x| \leq a, \\ \cos ka \exp[-\alpha(|x| - a)] & \text{if } |x| \geq a, \end{cases} \quad (22)$$

where $\Phi(y)$ is a smooth function which for the equivalent faces $y = -b$ and $y = b$ can be approximated by $\cos(\pi y / 2b)$. Substituting Eq. (22) into Eq. (20) and taking $o_x = 1, o_y = 0$ for the faces $x = \pm a$, we can derive the function h in the first approximation as

$$h(x,y) = C Q \sin \frac{\pi y}{2b} \begin{cases} \sin kx & \text{if } |x| \leq a, \\ \text{sgn}(x) \sin ka \exp[-\alpha(|x| - a)] & \text{if } |x| \geq a, \end{cases} \quad (23)$$

where

$$Q = \frac{\pi}{4kb} \frac{g_A(E) - g_B(E)}{\mu_A(E)} \cos^2 ka,$$

$\mu_A(E) = m_0 / m_A(E)$. Substituting f and h in the form of Eqs. (22) and (23) into Eq. (21), we finally obtain in the limit $b \rightarrow \infty$ the longitudinal g factor in the QW of the thickness $2a$:

$$g_{\parallel} = g_0 + G_A w_A (1 + \zeta_A \cos^2 ka) + G_B w_B (1 + \zeta_B \sin^2 ka), \quad (24)$$

where

$$\zeta_A = \frac{1}{2} \frac{g_B(E) - g_A(E)}{\mu_A(E)}, \quad \zeta_B = \frac{1}{2} \frac{g_A(E) - g_B(E)}{\mu_B(E)}.$$

The value of g_{\parallel} marked in Fig. 3 by the arrow is calculated by using Eq. (24); it coincides within the computational accuracy with values obtained by the previous methods.^{4,5}

VI. SUMMARY

We have studied consequences of the dimensionality reduction upon the Zeeman effect in semiconductor nanostructures and developed a theory of the electron Landé g factor of the lowest confined state in zinc-blende-based QWR's and QD's. For this purpose we have extended the approach used earlier to calculate the transverse g factor in QW's.⁵ Our concept allows us to obtain the g -factor components in one- and zero-dimensional systems avoiding the cumbersome summation over numerous quantum-confined electronic states. The further considerations have been carried out in the Kane model. The restrictions imposed by the structure symmetry have been analyzed and formulated. The effect of di-

mensionality has been demonstrated on spherical QD's and cylindrical QWR's. Compact analytical expressions have been derived for the electron g factor including the longitudinal g factor in QW's. The proposed theoretical scheme has been most completely realized by calculating the three different g -factor components in rectangular QWR's where the conduction-band spinor envelope $u(\boldsymbol{\rho})$ contains a spin-

dependent term and is characterized by two linearly independent scalar functions.

ACKNOWLEDGMENTS

This work was part of a research program financially supported by the Volkswagen Foundation and Russian Foundation for Basic Research.

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