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Electron effective g factor in small quantum systems

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Abstract. The Zeeman effect for 1D and 0D electron states has been considered theoretically. We have established the relation between the point symmetry of a low-dimensional system and properties of the g factor tensor $g_{\alpha\beta}$, from which, in particular, it turns out that the g factor in a cylindrical wire is isotropic ($g_{xx} = g_{yy} = g_{zz}$). The actual calculation of $g_{\alpha\beta}$ is performed for the ground states in rectangular quantum wire, cylindrical wire and spherical quantum dot structures.

Introduction

In zinc-blende semiconductors, the electron g factor values change with a chemical composition in a wide range ($g \approx 2$ in wide-gap semiconductors, -0.44 in GaAs and approximately -50 in the narrow-gap InSb). This behavior, i.e. dependence of g on the fundamental energy gap, E_g , and the spin-orbit splitting, Δ , of the upper valence band, is in a good agreement with the well-known Roth equation derived in the second order of the $\mathbf{k}\mathbf{p}$ perturbation theory. In [1] this approach was generalized to include heterostructures with quantum wells (QWs) and superlattices and the g factor was calculated as a function of layer widths. A large anisotropy of the Zeeman effect for conduction electrons was predicted, which was later confirmed experimentally in the structures grown from cubic semiconductors A_3B_5 and A_2B_6 (see [2] and references therein). First measurements of g factors for quantum dots have been reported more recently [3]. In the present work the theory of Zeeman effect for electrons in quasi-one- and quasi-zero-dimensional systems, namely quantum wires (QWRs) and quantum dots (QDs) is developed. The dependencies on the linear sizes are calculated for the g factor tensor in cylinder and rectangular QWRs as well as in a spherical QD.

1 The first- and second-order g factor formulae

As mentioned above, the expression for the g factor in bulk semiconductors comes from the second-order $\mathbf{k}\mathbf{p}$ perturbation theory. In this case a value of g is obtained as a sum over all intermediate states. In particular, for the electron in a simple band l of the bulk semiconductor of cubic symmetry with the extremum in the center of the Brillouin zone we have (magnetic field $\mathbf{B} \parallel z$)

$$g = g_0 + \sum_n \frac{|\langle l|p_+|n\rangle|^2 - |\langle l|p_-|n\rangle|^2}{E_l^0 - E_n^0}, \quad (1)$$

where $g_0 \approx 2$ is free electron Lande's factor, $\hat{p}_\pm = \hat{p}_x \pm i\hat{p}_y$, $\langle n|\hat{p}_\alpha|m\rangle$ ($\alpha = x, y, z$) is the matrix element of the momentum operator taken between states n and m , E_n^0 is the state electron energy. Here and in what follows we will use the atomic units with

the electronic charge $e = 1$, Plank's constant $\hbar = 1$ and the free-electron mass $m_0 = 1$. Though principally applicable to any types of semiconductor heterostructures, this approach involves calculation of intermediate states and, therefore, is very cumbersome and practically ineffective for one- and zero-dimensional systems. In this work we propose an approach which is much more suitable for g factor calculations in QWRs and QDs.

To begin with, we would like to mention, that the same result for g factor can be produced in the first order by the correction

$$\delta H = \frac{1}{c} \mathbf{A} \hat{\mathbf{V}}$$

to the electron Hamiltonian linear in the magnetic field, where \mathbf{A} is the vector-potential which in a homogeneous magnetic field depends linearly on the radius-vector \mathbf{r} , and the velocity operator $\hat{\mathbf{V}} = \partial H(\mathbf{k}) / \partial \mathbf{k}$. In order to show an equivalence of both approaches, one needs (1) to write the matrix element of the operator $\mathbf{A} \hat{\mathbf{V}}$ as a product of \mathbf{A} and $\hat{\mathbf{V}}$ matrix elements summed over intermediate states, and (2) to use a relation between the matrix elements of coordinate and velocity operators. Thus, we confirm that expressions for the g factor, produced in the second order of the $\mathbf{k}\mathbf{p}$ perturbation theory and in the first order by the correction δH are equivalent. For the extended states matrix elements of δH usually can not be directly evaluated, so as the second-order expression for the g factor should be used instead.

If the wave function is localized in one of the directions ζ due to spatial confinement, the calculation of the g factor in the magnetic field $\mathbf{B} \perp \zeta$ can be performed in the first order of the perturbation theory in the correction to the electron Hamiltonian. In particular, in the structure with a quantum dot, where the envelope wave function is localized in all three directions, the first-order perturbation theory can be applied and the tensor $g_{\alpha\beta}$ of g factors for the ground state of the spatial quantization $e1$ is defined by the expression

$$\frac{1}{2} \mu_B \sigma_{\alpha,ss'} (g_{\alpha\beta} - g_0) B_\beta = \langle e1, s | \delta H | e1, s' \rangle. \quad (2)$$

Here μ_B is the Bohr magneton, σ_α ($\alpha = x, y, z$) are the Pauli matrices, and the spin indices $s, s' = \pm 1/2$. Equation (2) is applicable as well for the electron state at the bottom of the subband $e1$ in a quantum wire, if (1) the vector potential gauge is chosen so as it depends only on the coordinates perpendicular to the wire axis and (2) the diamagnetic contribution is subtracted from the right-hand side of Eq. (2) [2]

$$\frac{1}{c} \langle e1, s | \hat{v}_z | e1, s' \rangle \langle A_z(\mathbf{r}) \rangle.$$

2 Kane model calculation

For the analysis of an electron g factor we use the Kane model. It takes into consideration $\mathbf{k}\mathbf{p}$ mixing of states in the conduction band Γ_6 and in the valence bands Γ_8, Γ_7 exactly, but neglects influence of the remote bands. The Schrödinger equation with the $\mathbf{k}\mathbf{p}$ Hamiltonian $H(\hat{\mathbf{k}})$ (matrix 8×8) can be written in terms of spinors u (conduction band, two components) and \mathbf{v} (valence band, six components) [4]. It is possible to

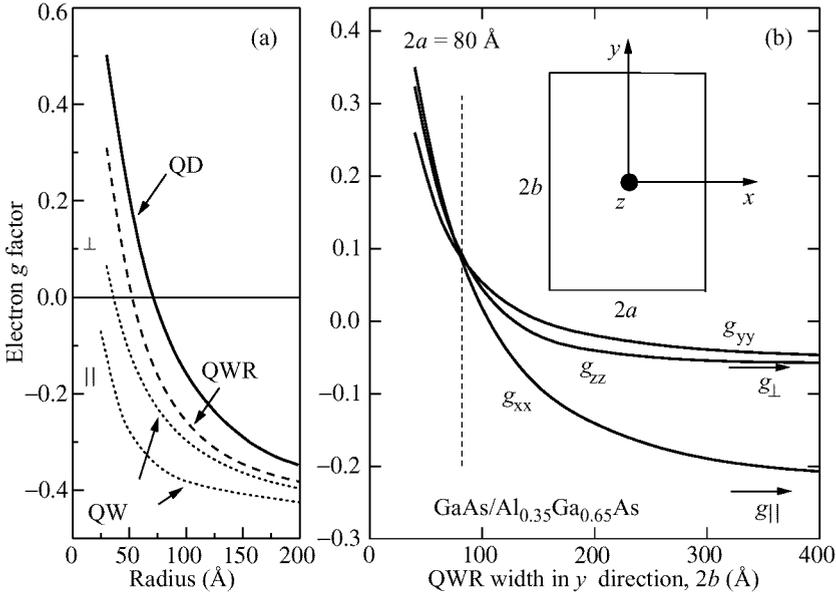


Fig 1. (a) Dependence of the electron g factor on the structure linear sizes. Values for the spherical QD and cylindrical QWR of radius R are presented by solid and dashed lines respectively. For comparison the longitudinal and transverse components of the electron g factor tensor ($g_{\parallel}^{QW} < g_{\perp}^{QW}$) are shown for the single QW of width $2R$ (dotted line). (b) The b -dependence of the electron g factor $g_{\alpha\beta}$ at the bottom of the first subband in GaAs/Al_{0.35}Ga_{0.65}As QWR with a cross-section $2a \times 2b$ (see inset). Dashed line marks a case of $a = b$. Arrows show longitudinal (g_{\parallel}) and transverse (g_{\perp}) g factor components in a 80 Å-wide QW.

reduce this system to a second-order differential equation

$$-\frac{P^2}{3} \left(\frac{2}{E_g + E} + \frac{1}{E_g + E + \Delta} \right) \nabla^2 u = E u, \tag{3}$$

for the spinor u , and the vector spinor \mathbf{v} can be expressed via the gradient ∇u by the equation

$$P\mathbf{v} = \frac{P^2}{3} \left[\left(\frac{2}{E_g + E} + \frac{1}{E_g + E + \Delta} \right) \nabla u + \frac{i\Delta}{(E_g + E)(E_g + E + \Delta)} (\boldsymbol{\sigma} \times \nabla u) \right]. \tag{4}$$

Here E is the electron energy counted from the conduction band bottom Γ_6 , and boundary conditions are the continuity of the spinor $u(\mathbf{r})$ and of the component of the vector $P\mathbf{v}(\mathbf{r})$ parallel to the interface normal, $P = i\langle S | \hat{p}_z | Z \rangle$.

In the Kane model the velocity operator $\hat{\mathbf{V}}$ is an 8×8 matrix with \mathbf{k} -independent components. Using an explicit form of this matrix, we conclude the section with the main formula for the g factor calculation

$$\langle e1, s | \delta H | e1, s' \rangle = i \frac{e}{\hbar} \int P [(\mathbf{A}\mathbf{v}_s^+) u_{s'} - u_s^+ (\mathbf{A}\mathbf{v}_{s'})] d\mathbf{r}. \tag{5}$$

3 Results and discussion

In Fig. 1a the electron g factor in a spherical QD (g^{QD}) and in a cylindrical QWR (g^{QWR}) are presented as a function of the radius R . For comparison in the same graph we show longitudinal (g_{\parallel}^{QW} , $\mathbf{B} \parallel z$) and transverse (g_{\perp}^{QW} , $\mathbf{B} \perp z$) g factor components for a QW of the width $2R$. The model calculation is performed for the heterosystem GaAs/Al_{0.35}Ga_{0.65}As. The following parameter values are used in the calculation: $E_g = 1.52$ eV, $\Delta = 0.34$ eV, $2p_{cv}^2/m_0 = 28.9$ eV for bulk GaAs ($p_{cv} = i\langle S|\hat{p}_z|Z\rangle$), and $E_g = 1.94$ eV, $\Delta = 0.32$ eV, $2p_{cv}^2/m_0 = 26.7$ eV for the barrier material, band offsets at the interface are $\Delta E_v:\Delta E_c = 2:3$. In order to take into account the contribution of remote bands we added a constant $\Delta g = -0.12$ to the g factor values obtained in the Kane model. Thus, with increasing the structure size the electron g factor reaches a bulk value of -0.44 in GaAs. With a decreasing the linear sizes the g factor increases tending for $R \rightarrow 0$ to the barrier material value 0.57 . Since with the reduction in the system dimensionality the role of spatial confinement increases, the following relations are fulfilled: $g_{\parallel,\perp}^{QW} < g^{QWR} < g^{QD}$.

Fig. 1b presents the tensor $g_{\alpha\beta}$ for an electron in the ground state in a rectangular QWR of the cross-section $2a \times 2b$ as a function of the length b . The other size ($2a = 80$ Å) is kept constant. For the square cross-section ($a = b$), the components g_{xx} and g_{yy} coincide the same, and the anisotropy $g_{zz} - g_{xx}$ is very small in agreement with the general symmetry considerations. With increasing b we asymptotically approach the QW limit resulting in $g_{xx} \rightarrow g_{\parallel}$ and $g_{xx}, g_{yy} \rightarrow g_{\perp}$, where g_{\parallel} and g_{\perp} are the longitudinal and transverse components of the g factor in a QW.

Thus, by using the Kane model we have developed a theory of the electron g factor in semiconductor QWRs and QDs, and performed model calculations for the spherical dot, rectangular and cylindrical wires.

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