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# Designing heterostructures with predefined value of light-hole $g$ factor for coherent solid-state quantum receiver

A.A. Kiselev[a,*], K.W. Kim[b], E. Yablonovitch[b]

[a] *Department of Electrical and Computer Engineering, North Carolina State University, Box 7911, Raleigh, NC 27695-7911, USA*
[b] *Department of Electrical Engineering, University of California, Los Angeles, Los Angeles, CA 90024, USA*

**Abstract**

In this paper, we give a consistent theoretical analysis of the in-plane Zeeman effect for quantum-confined light holes and evaluate possibilities to design structures with desired property of large $g$ factor for these valence states. Numerical example is given for the technologically important InGaAs/InP both lattice-matched and strained heterosystems suitable for 1.3 and 1.55 μm optoelectronic applications. © 2002 Elsevier Science B.V. All rights reserved.

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Secure quantum communication schemes are based on entanglement of coherent quantum states (see Ref. [1] and references therein). To achieve this for practical use, one must be able to transmit quantum information over long distances, perform elements of quantum computing to execute error correction, and retain the information without decoherence. Such rigorous conditions require development of a system that is capable of receiving quantum information in the form of coherent photon states, storing the information, performing the necessary operations, and then retransmitting the photon signal while maintaining quantum coherence throughout the process. It is well known that information in the form of photon polarization can be transferred to electron spin in semiconductors and vice versa in absorption/emission processes [2]. Hence, utilizing the electron spin degree of freedom in solids provides a clear pathway to the development of a practical quantum communication system. Such a system could reliably function as a repeater to transmit quantum information over long distances and would accomplish a number of goals, including, for example, secure data transmission.

A promising scheme, based on nanoscale semiconductor technology, was recently proposed to achieve this function [3]. The suggested quantum communication system resembles conventional optical communication systems except that it takes advantage of particular photon absorption/emission selection rules. The design of the proposed receiver (and transmitter) needs to satisfy several demanding conditions simultaneously, one of them requires that both electron sublevels should couple optically to a single ground hole state, thus excluding entanglement with the quickly relaxing hole spin. Application of an external magnetic field leads to the desired valence band splitting that should be sufficiently large to resolve hole

* Corresponding author. Tel.: +1-919-515-5080; fax: +1-919-515-3027.
*E-mail address:* kiselev@eos.ncsu.edu (A.A. Kiselev).


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sublevels spectroscopically. A proper experimental setup provides selection rules of the corresponding optical transitions that enable the transfer of photon polarization into the electron spin. This setup is thoroughly discussed in Ref. [3]; we follow those proposed selection rules and concentrate on the geometry with in-plane magnetic field and Zeeman splitting of the light-hole (LH) sublevels.

The free electron spin splitting factor, of value $g = 2.0023$ defines the influence of the external magnetic field on the doublet of otherwise degenerate electron states with spin $s = \pm\frac{1}{2}$. Interaction of electron states with the lattice potential in crystals (and superpotential in heterostructures) leads to the (often strong) renormalization of the $g$ factor value [4–6].

No work has been done for the LH states to the best of the authors knowledge. That is due, in part, to the fact that the much smaller effective mass and resulting higher quantization energies (compared to those for HHs) make it difficult even to detect LH states in typical heterostructures. Applied or lattice-mismatch-induced intrinsic strain can reverse this situation making LH the ground hole state in the structure with a QW.

The general approach to calculate $g$ factor for a pair of Kramers-degenerate states in a heterostructure has already been described in the literature [6]. The main result of the derivation is summarized as follows: let us consider a multiband Hamiltonian $H(\boldsymbol{k})$ in the presence of external magnetic field $\boldsymbol{B} = \nabla \times \boldsymbol{A}$. The procedure suggests two replacements $\boldsymbol{k} \to \boldsymbol{k} + \boldsymbol{A}/c$ (implicit magnetic field dependence, through vector potential) and Hamiltonian $H \to H + \delta H_{\boldsymbol{B}}$ (explicit term, describing direct interaction with the magnetic field in the chosen model). Hereafter, we use the atomic units.

For a pair of states $|s\rangle$ ($s = \uparrow$ or $\downarrow$), the Zeeman contribution to the effective $2 \times 2$ Hamiltonian can be written as

$$\delta\mathscr{H}_{ss'} \equiv \frac{1}{4c}\sigma_{\alpha,ss'}g_{\alpha\beta}B_\beta = \frac{1}{c}\left\langle s\left|\boldsymbol{A}\frac{\partial H}{\partial \boldsymbol{k}}\right|s'\right\rangle + \langle s|\delta H_{\boldsymbol{B}}|s'\rangle, \quad (1)$$

where $\hat{\sigma}_\alpha$ are the Pauli matrices, $1/4c$ stands for the half of the Bohr magneton $\mu_B/2$ in atomic units. Eq. (1) can be considered as a definition of the $g$ factor tensor with real components $g_{\alpha\beta}$.

Thus, in order to calculate the tensor $g_{\alpha\beta}$ it suffices to choose an adequate multiband $\boldsymbol{kp}$ model and find, first, the envelope functions $\varphi_n$ in the multicomponent expansion $|s\rangle = \sum_n \varphi_n(\boldsymbol{r})|n\rangle$ in the semiconductor structure at zero magnetic field and, second, evaluate the required matrix elements $\int \mathrm{d}\boldsymbol{r}\ \varphi_n^*(\boldsymbol{r})\{\boldsymbol{A}\partial H/\partial \boldsymbol{k}\}_{nn'}\varphi_{n'}(\boldsymbol{r})$, $\int \mathrm{d}\boldsymbol{r}\ \varphi_n^*(\boldsymbol{r})\delta H_{\boldsymbol{B},nn'}\varphi_{n'}(\boldsymbol{r})$ where the integration is performed separately over all structure domains bounded by interfaces. The ability to evaluate directly these matrix elements depends on the proper choice of the vector potential gauge. For the quantized state in the QW with the growth direction $z$, the vector potential for the in-plane magnetic field should be taken in the form $A(z) = (B_y z, -B_x z, 0)$. We stress that here $n$ is the index enumerating only the electronic bands in the constituent bulk semiconductors, not numerous individual quantum states.

Analyzing merits and shortcomings of the various model Hamiltonians, we concluded to use the complete $8 \times 8$ $\boldsymbol{kp}$ Hamiltonian [7,8] in the hole $g$ factor calculations, which takes the interaction of the $\Gamma_6$, $\Gamma_8$, and $\Gamma_7$ bands exactly into account (like the model of Kane [9]) and does not omit the contributions of the remote bands by keeping them in a quadratic-in-$\boldsymbol{k}$ approximation (similar to the Luttinger–Kohn approach [10]). Fig. 1 graphically presents involved band structure parameters and $\boldsymbol{kp}$ interactions for a typical III–V semiconductor. The matrix elements of the utilized bulk $8 \times 8$ Hamiltonian are given in the appendix of Ref. [8].

The LH wave function $|\uparrow\rangle$ in QW at the bottom of the subband ($k_x = k_y = 0$) can be written in the form

$$|\uparrow\rangle = u(z)|S\uparrow\rangle + v(z)|\mathrm{LH}\uparrow\rangle + w(z)|\mathrm{SO}\uparrow\rangle, \quad (2)$$

where $u, v, w$ are conduction band, LH, and SO $z$-dependent envelopes, respectively, $|j\rangle$ are the Bloch amplitudes. The set of functions $(u, v, -w)$ defines $|\downarrow\rangle$. HH states do not mix into functions $|\uparrow\rangle$, $|\downarrow\rangle$ at the bottom of the subband, simplifying derivations considerably.

Our general procedure gives for the in-plane component of the LH $g$ factor

$$g_{\mathrm{LH},\perp} = g_{\mathrm{imp}} + g_{\mathrm{exp}}, \quad (3)$$

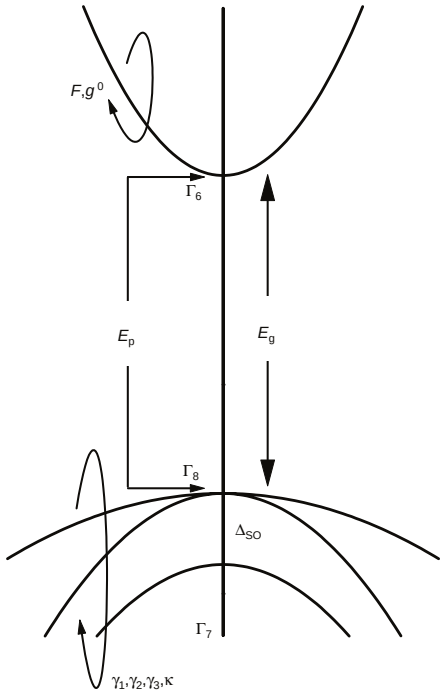


Fig. 1. Band diagram of a typical III–V semiconductor. $E_g$ is the band gap, $\Delta$ is the spin–orbit splitting of the $\Gamma_8$ and $\Gamma_7$ bands, the $E_p$ parameter is related to the interband matrix element of the angular momentum operator through $E_p = 2P^2$, and the parameter $F$ determines the conduction band curvature due to the interaction with the remote bands. The modified Luttinger parameters $\gamma_1$, $\gamma_2$, $\gamma_3$, and $\kappa$ describe the effect of the remote bands on the $(\Gamma_8+\Gamma_7)$ valence band of the semiconductor and can be expressed through the standard Luttinger constants $\gamma_i^{\mathrm{L}}$ and $\kappa^{\mathrm{L}}$. The parameter $q$, determining the cubic-in-$\boldsymbol{J}$ valence-band spin splitting, is small and, hence, is dropped here. For simplicity we also assume that quadratic-in-$\boldsymbol{k}$ term $(F+\frac{1}{2})$ is zero and $g^0$ is equal to the Landè factor of free electrons ($\approx 2$).

where $g_{\mathrm{imp}}$ is a result of evaluation of the first, vector-potential-related term in Eq. (1),

$$g_{\mathrm{imp}} = 4\int \mathrm{d}z\, z\left[\frac{3}{\sqrt{2}}\gamma_3(w^*v' - v^*w') + \frac{E_{\mathrm{p}}}{3(E_g - E)} \times \left(v^*v' - \frac{1}{\sqrt{2}}v^*w' + \sqrt{2}w^*v' - w^*w'\right)\right], \quad (4)$$

while $g_{\mathrm{exp}}$ comes from the second term responsible for the direct interaction with the magnetic field

$$g_{\mathrm{exp}} = 4\int \mathrm{d}z\left[\frac{1}{2}|u|^2 - \kappa|v|^2 + \left(\kappa + \frac{1}{2}\right)|w|^2 - \frac{1}{\sqrt{2}}(\kappa+1)(v^*w + w^*v)\right]. \quad (5)$$

The theory developed thus far is equally applicable to any cubic semiconductor with a band structure similar to that shown in Fig. 1. This includes both III–V and II–VI pure compounds and solid solutions. With the strain-induced energy shifts included, wurtzite crystals can be analyzed as well in the framework of the quasi-cubic model that treats wurtzite crystal as a strained cubic one. In our analysis, we assume the structure to be grown pseudomorphically on an unstrained substrate. The choice of the substrate composition defines the common in-plane lattice constant $a_{\mathrm{sub}}$ and, consequently, strains in the heterostructure layers. Shifts of the conduction and valence band edges due to the strain are defined by the deformation potentials and are incorporated into the calculation procedure [11].

For illustration, we use here the most widely utilized $In_{1-x}Ga_xAs/InP$ heterosystem. However, we decided to prepare our numerical procedure and data, so as they are readily applicable to structures with both well and barrier materials based on the (more general) quaternary solid solutions $In_{1-x}Ga_xAs_yP_{1-y}$, which are useful for 1.3 and 1.55 μm optoelectronic applications. Band structure parameters for constituent pure compounds can be found in Ref. [12]. We use an interpolation scheme for the solutions with different $(x, y)$ compositions. For the band gap we apply an equation given in Ref. [12] (with a proper adjustment for the low-temperature regime)

$$E_g = 1.424 + 0.713x - 1.084y + 0.758x^2 + 0.078y^2 - 0.078xy - 0.322x^2y + 0.03xy^2 \text{ (in eV)}. \quad (6)$$

For other parameters of the band structure ($\Delta, E_{\mathrm{p}}$, modified—only remote band contributions—Luttinger parameters $\gamma_i, \kappa$) we apply bilinear interpolation of values for pure semiconductors.

Fig. 2 presents calculated $g$ factor values for a free (not bound in the exciton or localized) LH in the unstrained as well as strained InGaAs/InP heterostructures as a function of the InGaAs layer thickness. We repeat, that the orientation of the applied magnetic

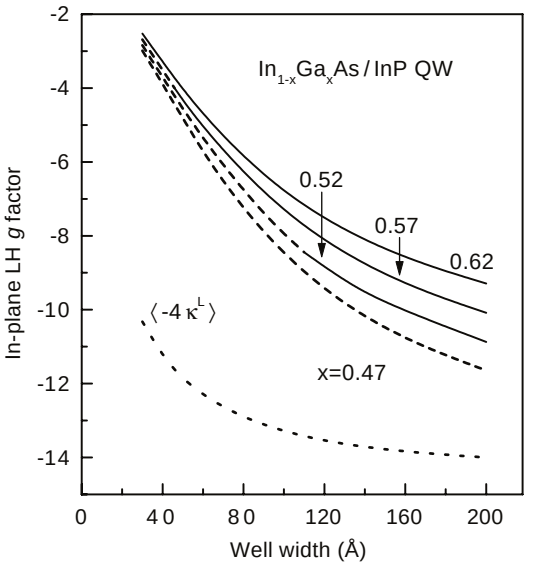


Fig. 2. The in-plane LH $g$ factor in $In_{1-x}Ga_xAs/InP$ QW as a function of the well layer width. Solid and dashed lines present results of the calculation. Depending on the QW width and intrinsic strain defined by the InGaAs layer composition $x$, either HH or LH subband acts as a ground hole state in the QW, this information is delivered by the line type: dashed and solid, respectively. Dotted line visualizes naive approach based on the averaging of the material-dependent Luttinger parameter $\kappa^L(E)$ ("bulk" in-plane LH $g$ factor) with probabilities to find the hole in the well and barrier layers.

field was assumed to be in-plane. The calculation was carried out for the hole states at the bottom of the LH subband in the single QW structure. Both solid and dashed curves are produced using the procedure outlined above; a solid line is used when the LH forms the ground hole state while the dashed line is used otherwise. Depending on the concurrent effects of the strain caused by the lattice constant mismatch and the quantum confinement, either LHs or HHs form the ground hole states. In very wide wells, strain alone defines the order of levels. If the effects of strain and confinement are opposite in sign, a cross-over in the character of the ground state happens at some intermediate well width, below which the effect of confinement prevails. We emphasize again that we are primarily interested in the structure with the ground hole state formed by the LH. Our calculation gives dependencies that are steep at small layer thicknesses, but asymptotically approach their respective "bulk" values for very wide QWs. Though not explicitly present in Fig. 2, at very narrow well widths (where the applicability of the macroscopic ***kp*** method itself can probably be questioned) the in-plane LH $g$ factor crosses zero for our heteropair choice. In this case, there will be no Zeeman splitting of the spin-up and spin-down LH states. For the purposes of the quantum receiver [3], one should avoid this region of well widths. Indeed, the $g$ factor should be kept at a reasonably large value, which we have shown is feasible for a broad range of structure widths.

Results of the unsophisticated approach, meaning simple averaging of the (energy-dependent) "bulk" in-plane values for LHs with quantum-mechanical probabilities to find particle in different heterolayers, is also given in Fig. 2 as the dotted line. By no means simple averaging can be considered as a satisfactory procedure.

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