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2003 J. Phys.: Condens. Matter 15 L67

(http://iopscience.iop.org/0953-8984/15/2/109)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS: CONDENSED MATTER

J. Phys.: Condens. Matter **15** (2003) L67–L75 PII: S0953-8984(03)36545-2

**LETTER TO THE EDITOR**

# $k \cdot p$ Hamiltonians for quantum dots in a magnetic field

**J Planelles**[1] **and W Jaskólski**[2]

[1] Departament de Ciències Experimentals, UJI, Box 224, E-12080 Castelló, Spain
[2] Instytut Fizyki UMK, Grudziądzka 5, 87-100 Toruń, Poland

E-mail: planelle@exp.uji.es and wj@phys.uni.torun.pl

Received 2 May 2002
Published 6 January 2003
Online at stacks.iop.org/JPhysCM/15/L67

**Abstract**

The problem of multiband $\boldsymbol{k} \cdot \boldsymbol{p}$ Hamiltonians describing the hole energy structure of semiconductor nanosystems in a magnetic field is addressed. The approximate formulation given previously by Luttinger [1] is revisited. We show that interaction with a magnetic field enters into the multiband equations for the envelope function components through the usual quadratic term and two linear Zeeman terms. The first linear term corresponds to the envelope angular momentum, while the other corresponds to the Bloch band-edge angular momentum. Several approximate ways of including the magnetic field in a four-band valence Hamiltonian are discussed and numerically compared.

The influence of a magnetic field on the electronic and optical properties of zero-dimensional semiconductor nanostructures has been intensively studied for the last two decades [2, 3]. The weaker quantum confinement and lighter electron effective mass than in atomic physics has the result that in a strong magnetic field the energy of interaction with the field may exceed the confinement energies and lead to the observation of effects that, for natural atoms would require fields many orders of magnitude stronger than those accessible in the laboratory. The vast majority of work has been devoted to investigating the energy structure of the conduction band electrons. In such a case one usually solves the one-band effective mass equation for a charged particle in a magnetic field. The Hamiltonian of such system is:

$$H = \frac{1}{2m}(\boldsymbol{p} - e\boldsymbol{A})^2 + V(\boldsymbol{r}), \tag{1}$$

where $\boldsymbol{A}$ is the vector potential of the magnetic field $\boldsymbol{B}$ and $V(\boldsymbol{r})$ is a confining potential. When $\boldsymbol{B}$ is applied in the $z$-direction and the symmetric gauge, $\nabla \cdot \boldsymbol{A} = 0$, is used for $\boldsymbol{A} = (-\frac{1}{2}y, \frac{1}{2}x, 0)B$, the Hamiltonian becomes:

$$H = \frac{\boldsymbol{p}^2}{2m} - \frac{e}{m}\boldsymbol{A} \cdot \boldsymbol{p} + \frac{e^2}{2m}\boldsymbol{A}^2 + V(\boldsymbol{r}) = \frac{\boldsymbol{p}^2}{2m} - \frac{eB}{2m}\hat{L}_z + \frac{e^2B^2}{8m}\rho^2 + V(\boldsymbol{r}). \tag{2}$$

0953-8984/03/020067+09$30.00  

In the one-band approximation the wavefunction $\Psi$ is just a product of the envelope function $f(\boldsymbol{r})$ and the Bloch function $|u\rangle = |S\rangle\sigma$, with $\sigma = \alpha$ or $\beta$ and $|S\rangle$ being a spherically symmetric Bloch function.

When interaction with the remote bands is included, $m$ is replaced by the effective mass $m^*$. If the confining potential has axial (or spherical) symmetry the variables in the envelope function separate, $f(\rho, z, \phi) = \frac{1}{\sqrt{2\pi}} e^{iM\phi}\Phi(\rho, z)$, where $M$ is the quantum number of $\hat{L}_z$. Left-multiplying $H\Psi$ by $\langle u|$, integrating over the unit cell and over $\phi$ yields

$$\left[\frac{p^2}{2m^*} - \frac{eBM}{2m^*} + \frac{e^2B^2}{8m^*}\rho^2 + V(\rho, z) - E\right]\Phi(\rho, z) = 0, \tag{3}$$

where we have employed $\hat{L}_z|S\rangle = 0$ and thus $\langle u|\hat{L}_z(|u\rangle|f\rangle) = \langle u|u\rangle\hat{L}_z|f\rangle = \hat{L}_z|f\rangle$.

A two-dimensional version of this equation with a parabolic confining potential $V(\rho) = \frac{1}{2}m^*\omega^2\rho^2$ is known as the Darwin–Fock equation and has so far been most frequently used to model quasi-two-dimensional quantum dots. Equation (3) has also been used to investigate the electron energy structure of spherical multilayer nanocrystals [4–6] and quantum dot rings [7, 8].

The inclusion of the electron spin will lead to two additional terms: the spin Zeeman energy $g\mu_B\sigma B$ (where $g$ is the gyromagnetic factor and $\mu_B$ is the Bohr magneton) describing the interaction of the spin with the magnetic field, and the spin–orbit term. The spin–orbit term is usually neglected, since the conduction band is built of atomic s-type orbitals which makes this interaction weak [2].

The valence-band energy structure of a given semiconductor nanosystem cannot be properly described by a simple one-band effective mass equation. In such a case one has to consider multiband $\boldsymbol{k}\cdot\boldsymbol{p}$ Hamiltonians that allow for valence subband mixing. In the most general case, i.e., when there are $N$ degenerate or energetically close bands, the one-electron wavefunction in the envelope function approximation (EFA) is represented by:

$$\Psi(\boldsymbol{r}) = \sum_i^N u_i f_i(\boldsymbol{r}), \tag{4}$$

where $u_i$ are the Bloch band-edge functions and $f_i$ are the envelope function components [9].

To obtain the set of coupled differential equations (in a given $\boldsymbol{k}\cdot\boldsymbol{p}$ model) for the envelope components one has to apply the one-particle Hamiltonian, equation (1), upon the wavefunction (4), left-multiply by $u_j$ and integrate over the unit cell. In the eight-band model (the one most widely used for the narrow-gap semiconductors), which couples the conduction, heavy-hole, light-hole and split-off bands, the $u_i$ are usually chosen as the conventional Luttinger–Kohn basis [9, 10] $|(c/v), J, J_z\rangle$ ($J$ is the Bloch angular momentum and $c/v$ means conduction/valence band)

$$\begin{aligned}
&|c, \tfrac{1}{2}, \tfrac{1}{2}\rangle = |S\rangle\alpha \\
&|c, \tfrac{1}{2}, -\tfrac{1}{2}\rangle = |S\rangle\beta \\
&|v, \tfrac{3}{2}, \tfrac{3}{2}\rangle = -1/\sqrt{2}|P_+\rangle\alpha \\
&|v, \tfrac{3}{2}, \tfrac{1}{2}\rangle = \sqrt{2/3}|Z\rangle\alpha - 1/\sqrt{6}|P_+\rangle\beta \\
&|v, \tfrac{3}{2}, -\tfrac{1}{2}\rangle = \sqrt{2/3}|Z\rangle\beta + 1/\sqrt{6}|P_-\rangle\alpha \\
&|v, \tfrac{3}{2}, -\tfrac{3}{2}\rangle = 1/\sqrt{2}|P_-\rangle\beta \\
&|v, \tfrac{1}{2}, \tfrac{1}{2}\rangle = 1/\sqrt{3}|P_+\rangle\beta + 1/\sqrt{3}|Z\rangle\alpha \\
&|v, \tfrac{1}{2}, -\tfrac{1}{2}\rangle = -1/\sqrt{3}|P_-\rangle\alpha + 1/\sqrt{3}|Z\rangle\beta
\end{aligned} \tag{5}$$

where $\alpha$, $\beta$ are the spin functions, $|P_+\rangle = |X\rangle + \mathrm{i}|Y\rangle$, $|P_-\rangle = (|X\rangle - \mathrm{i}|Y\rangle)$ and $|X\rangle$, $|Y\rangle$, $|Z\rangle$ are the basis functions of the $\Gamma_8$ representation.

To check how the magnetic field influences the multiband $\boldsymbol{k}\cdot\boldsymbol{p}$ equations for the envelope components, we first apply the one-particle Hamiltonian (2) upon the wavefunction (4), left-multiply by $u_j$ and integrate over the unit cell. Then, evaluate $\langle u_j|W(|u_i\rangle|f_i\rangle)$, where $|u_i\rangle$ belongs to the above basis set, equation (5), and $W$ is the magnetic interaction term in the one-particle Hamiltonian (2):

$$W = -\frac{eB\hat{L}_z}{2m} + \frac{e^2B^2}{8m}\rho^2. \tag{6}$$

The second (quadratic) term of equation (6) is purely multiplicative and is thus diagonal. The integration over the unit cell in $\langle u_j|\hat{L}_z(|u_i\rangle|f_i\rangle)$ yields,

$$\langle u_j|\hat{L}_z(|u_i\rangle|f_i\rangle) = \langle u_j|\hat{L}_z|u_i\rangle|f_i\rangle + \delta_{ij}\hat{L}_z|f_i\rangle. \tag{7}$$

Let us note, that the second term of equation (7) is also always diagonal. Consider now the first term of equation (7). Since $\hat{L}_z|S\rangle = 0$, $\hat{L}_z|Z\rangle = 0$ and $\hat{L}_z|P_\pm\rangle = \pm|P_\pm\rangle$, one can easily see, that the only non-diagonal terms are those coupling $|v, \frac{3}{2}, \frac{1}{2}\rangle$ and $|v, \frac{1}{2}, \frac{1}{2}\rangle$, on the one hand, and $|v, \frac{3}{2}, -\frac{1}{2}\rangle$ and $|v, \frac{1}{2}, -\frac{1}{2}\rangle$, on the other hand. The value of $c_{ij} = \langle u_j|L_z|u_i\rangle$ equals $\frac{1}{3\sqrt{2}}$ in these two cases. The diagonal $c_{ii} = c_i$ factors are $\{0, 0, \frac{1}{2}, \frac{1}{6}, -\frac{1}{6}, -\frac{1}{2}, \frac{1}{3}, -\frac{1}{3}\}$ for the consecutive subbands in equation (5). It is important to note that, in our formulation, non-diagonal Zeeman terms appear only when the split-off band is present in the basis set, equation (5), and such non-diagonal terms are always linear.

Let us now consider the special case of the 4-band valence Hamiltonian coupling only the heavy-hole and light-hole subbands. If the investigated system has axial symmetry, i.e. if $V(\boldsymbol{r}) = V(\rho, z)$, as it is the case of a magnetic field applied to spherical nanocrystals, then the Hamiltonian commutes with the $z$-component $\boldsymbol{F_z}$ of the total angular momentum $\boldsymbol{F} = \boldsymbol{J} + \boldsymbol{L}$, where $\boldsymbol{L}$ is the envelope angular momentum and $\boldsymbol{J}$ is the Bloch band-edge angular momentum [10] ($J = 3/2$ for the heavy and light holes bands). The axial symmetry also allows us to write the envelope function components as: $f_i(\rho, z, \phi) = \frac{1}{\sqrt{2\pi}}\mathrm{e}^{\mathrm{i}(F_z - M_i)\phi} f_i(\rho, z)$, where $M_i$ are the quantum numbers of the $z$-components of the Bloch angular momentum of the consecutive bands in question. In this case the magnetic interaction term is totally diagonal:

$$\langle u_i|\hat{L}_z(|u_i\rangle|f_i\rangle) = (F_z - M_i)|f_i\rangle + c_i|f_i\rangle \tag{8}$$

and the magnetic field contribution to the resulting $\boldsymbol{k}\cdot\boldsymbol{p}$ Hamiltonian is also fully diagonal. Let us note, that in the approximation formulated originally by Luttinger [1] and used next by Pacheco *et al* [11], the magnetic interaction in a 4-band Hamiltonian is not diagonal. Later we discuss the relationship between these two formulations. When finally the interaction with remote bands is included, the magnetic interaction term (in au) is

$$\mathcal{W}_i = -\frac{(F_z - M_i)B}{2m^*} - \frac{c_iB}{2m^*} - \frac{B^2\rho^2}{8m^*}, \tag{9}$$

where $m^*$ is the absolute value of the heavy-hole or light-hole effective mass[3]. The last term accounts for the usual quadratic effect. Since $(F_z - M_i)$ is equal to the $z$-component of the envelope angular momentum, the first term of equation (9) is the orbital linear Zeeman effect for the effective hole. It describes the influence of a magnetic field on the global properties of the band-edge holes in a given zero-dimensional system. The second term corresponds to

[3] In the present letter we use $(\gamma_1 \pm 2\gamma)^{-1}$ as the HH and LH effective masses, with $\gamma_1$ and $\gamma$ being the Luttinger parameters. However, as it can be seen in table 1, the mass coefficients in front of $\rho$ and $z$ derivatives are different. We are currently exploring a possibility of using $(\gamma_1 \pm \gamma)^{-1}$ or some average values as the magnetic field mass coefficients.

the *internal* (or *local*) linear Zeeman effect associated with the Bloch angular momentum. It describes the influence of the magnetic field on the local (in the unit cell) properties of the valence-band holes. Hereafter we refer to the $4 \times 4$ Hamiltonian, including the magnetic terms, as $\mathcal{H}_{ex}$. This Hamiltonian, written in cylindrical coordinates and for $B = 0$ is shown in table 1. The magnetic interaction terms $\mathcal{W}_i$ are collected in table 2(a).

Since the multiband envelope equations describe the global properties of the holes in a given zero-dimensional semiconductor system under the influence of a magnetic field, the *local* Zeeman term should be, in principle, smaller than the *global* one. The approximate Hamiltonian with the second term in $\mathcal{W}_i$ neglected is called $\mathcal{H}_{gl}$. The (approximate) magnetic terms of $\mathcal{H}_{gl}$ are collected in table 2(b). Yet another approximation has been employed in [4] and [7] where the values $(F_z - M_i) + c_i$ are averaged, i.e. replaced by $F_z$ (see table 2(c)). We call the corresponding Hamiltonian $\mathcal{H}_{av}$.

Let us now discuss the relationship between the present derivation of the magnetic interactions within the 4-band model and the approximation introduced originally by Luttinger [1] and recently used by Pacheco *et al* [11]. In that approximation the interaction with the magnetic field is added after the $\boldsymbol{k} \cdot \boldsymbol{p}$ and EFA are applied, while in our formulation the interaction with a magnetic field is present already in the one-particle Hamiltonian (2). In [11] the components of $\vec{p}$ are replaced according to $\vec{p} \to \vec{p} - e\vec{A}$ in the original $\boldsymbol{k} \cdot \boldsymbol{p}$ EFA Hamiltonian [9, 10]

$$\begin{bmatrix} -(P+Q) & -\mathrm{i}L & -M & 0 \\ \mathrm{i}L^* & -(P-Q) & 0 & -M \\ -M^* & 0 & -(P-Q) & \mathrm{i}L \\ 0 & -M^* & -\mathrm{i}L^* & -(P+Q) \end{bmatrix} \tag{10}$$

where

$$P = \frac{\gamma_1}{2}p^2, \qquad Q = \frac{\gamma}{2}(p_\perp^2 - 2p_z^2), \qquad L = -\mathrm{i}\sqrt{3}\gamma_3 p_z p_-, \qquad M = \frac{\sqrt{3}\gamma}{2}p_-^2, \tag{11}$$
$$p_\pm = p_x \pm \mathrm{i}p_y, \qquad p_\perp^2 = p_x^2 + p_y^2, \qquad p^2 = p_\perp^2 + p_z^2, \qquad p_\alpha = -\mathrm{i}\nabla_\alpha,$$

$\gamma, \gamma_1, \gamma_3$ are Luttinger parameters ($\gamma_3 = \gamma$ in the spherical approximation), $\alpha = x$, $y$ or $z$, and $u_i$ are the Bloch functions.

One has to remember that $\vec{p}$ in equation (10) acts only on the envelope part of the wavefunction. It has a meaning of momentum, but is not equivalent to the momentum operator in the Hamiltonian (1).

After the replacement $\vec{p} \to \vec{p} - e\vec{A}$, i.e.

$$\begin{aligned} p_x &\to p_x - 1/2yB \\ p_y &\to p_y + 1/2xB \\ p_z &\to p_z, \end{aligned} \tag{12}$$

the Hamiltonian is transformed to cylindrical coordinates $(\rho, z, \phi)$. The integration over $\phi$ yields a set of four coupled differential equations in two variables $(\rho, z)$. The resulting Hamiltonian, $\mathcal{H}_L$ is shown in table 3.

At a first sight, $\mathcal{H}_L$ (see table 3) differs significantly from $\mathcal{H}_{ex}$ (and thus from the Hamiltonians $\mathcal{H}_{gl}$ and $\mathcal{H}_{av}$): the magnetic interaction is not diagonal in $\mathcal{H}_L$. However, a closer inspection reveals that they are not very different. In order to see the relationship between them, let us consider the determinant of a $4 \times 4$ matrix

$$\begin{bmatrix} a-x & 0 & c & 0 \\ 0 & b-x & 0 & c \\ c & 0 & b-x & 0 \\ 0 & c & 0 & a-x \end{bmatrix} \tag{13}$$

**Table 1.** Four-band $\boldsymbol{k}\cdot\boldsymbol{p}$ EFA valence Hamiltonian in cylindrical coordinates for $B = 0$ T.

| | | | |
|---|---|---|---|
| $\frac{(\gamma+\gamma_1)}{2}\left[\frac{\partial^2}{\partial\rho^2}+\frac{1}{\rho}\frac{\partial}{\partial\rho}-\frac{(F_z-1.5)^2}{\rho^2}\right]$ $+\frac{(\gamma_1-2\gamma)}{2}\frac{\partial^2}{\partial z^2}+V(\rho,z)$ | $\sqrt{3}\gamma_3\left[\frac{\partial^2}{\partial\rho\partial z}+\frac{F_z-0.5}{\rho}\frac{\partial}{\partial z}\right]$ | $-\sqrt{3}\frac{\gamma}{2}\left[\frac{\partial^2}{\partial\rho^2}+\frac{2F_z}{\rho}\frac{\partial}{\partial\rho}\right.$ $\left.+\frac{F_z(F_z-1)-0.75}{\rho^2}\right]$ | 0 |
| $\sqrt{3}\gamma_3\left[\frac{\partial^2}{\partial\rho\partial z}-\frac{F_z-1.5}{\rho}\frac{\partial}{\partial z}\right]$ | $\frac{(\gamma_1-\gamma)}{2}\left[\frac{\partial^2}{\partial\rho^2}+\frac{1}{\rho}\frac{\partial}{\partial\rho}-\frac{(F_z-0.5)^2}{\rho^2}\right]$ $+\frac{(\gamma_1+2\gamma)}{2}\frac{\partial^2}{\partial z^2}+V(\rho,z)$ | 0 | $-\sqrt{3}\frac{\gamma}{2}\left[\frac{\partial^2}{\partial\rho^2}+\frac{2(F_z+1)}{\rho}\frac{\partial}{\partial\rho}\right.$ $\left.+\frac{F_z(F_z+1)-0.75}{\rho^2}\right]$ |
| $-\sqrt{3}\frac{\gamma}{2}\left[\frac{\partial^2}{\partial\rho^2}-\frac{2(F_z-1)}{\rho}\frac{\partial}{\partial\rho}\right.$ $\left.+\frac{F_z(F_z-1)-0.75}{\rho^2}\right]$ | 0 | $\frac{(\gamma_1-\gamma)}{2}\left[\frac{\partial^2}{\partial\rho^2}+\frac{1}{\rho}\frac{\partial}{\partial\rho}-\frac{(F_z+0.5)^2}{\rho^2}\right]$ $+\frac{(\gamma_1+2\gamma)}{2}\frac{\partial^2}{\partial z^2}+V(\rho,z)$ | $-\sqrt{3}\gamma_3\left[\frac{\partial^2}{\partial\rho\partial z}+\frac{F_z+1.5}{\rho}\frac{\partial}{\partial z}\right]$ |
| 0 | $-\sqrt{3}\frac{\gamma}{2}\left[\frac{\partial^2}{\partial\rho^2}-\frac{2F_z}{\rho}\frac{\partial}{\partial\rho}\right.$ $\left.+\frac{F_z(F_z+1)-0.75}{\rho^2}\right]$ | $-\sqrt{3}\gamma_3\left[\frac{\partial^2}{\partial\rho\partial z}-\frac{F_z+0.5}{\rho}\frac{\partial}{\partial z}\right]$ | $\frac{(\gamma+\gamma_1)}{2}\left[\frac{\partial^2}{\partial\rho^2}+\frac{1}{\rho}\frac{\partial}{\partial\rho}-\frac{(F_z+1.5)^2}{\rho^2}\right]$ $+\frac{(\gamma_1-2\gamma)}{2}\frac{\partial^2}{\partial z^2}+V(\rho,z)$ |

**Table 2.** Diagonal magnetic interaction terms $\mathcal{W}_i$ corresponding to different $\boldsymbol{k}\cdot\boldsymbol{p}$ EFA Hamiltonians: (a) $\mathcal{H}_{ex}$, (b) $\mathcal{H}_{gl}$ and (c) $\mathcal{H}_{av}$.

| | | | | |
|---|---|---|---|---|
| (a) | $-(\gamma_1-2\gamma)\left[\frac{B^2\rho^2}{8}+\frac{(F_z-1)B}{2}\right]$ | $-(\gamma_1+2\gamma)\left[\frac{B^2\rho^2}{8}+\frac{(F_z-\frac{1}{3})B}{2}\right]$ | $-(\gamma_1+2\gamma)\left[\frac{B^2\rho^2}{8}+\frac{(F_z+\frac{1}{3})B}{2}\right]$ | $-(\gamma_1-2\gamma)\left[\frac{B^2\rho^2}{8}+\frac{(F_z+1)B}{2}\right]$ |
| (b) | $-(\gamma_1-2\gamma)\left[\frac{B^2\rho^2}{8}+\frac{(F_z-1.5)B}{2}\right]$ | $-(\gamma_1+2\gamma)\left[\frac{B^2\rho^2}{8}+\frac{(F_z-0.5)B}{2}\right]$ | $-(\gamma_1+2\gamma)\left[\frac{B^2\rho^2}{8}+\frac{(F_z+0.5)B}{2}\right]$ | $-(\gamma_1-2\gamma)\left[\frac{B^2\rho^2}{8}+\frac{(F_z+1.5)B}{2}\right]$ |
| (c) | $-(\gamma_1-2\gamma)\left[\frac{B^2\rho^2}{8}+\frac{F_zB}{2}\right]$ | $-(\gamma_1+2\gamma)\left[\frac{B^2\rho^2}{8}+\frac{F_zB}{2}\right]$ | $-(\gamma_1+2\gamma)\left[\frac{B^2\rho^2}{8}+\frac{F_zB}{2}\right]$ | $-(\gamma_1-2\gamma)\left[\frac{B^2\rho^2}{8}+\frac{F_zB}{2}\right]$ |

**Table 3.** Four-band $\mathcal{H}_L$ Hamiltonian.

| | | | |
|---|---|---|---|
| $\frac{(\gamma+\gamma_1)}{2}\left[\frac{\partial^2}{\partial\rho^2}+\frac{1}{\rho}\frac{\partial}{\partial\rho}-\frac{(F_z-1.5+0.5B\rho^2)^2}{\rho^2}\right]+\frac{(\gamma_1-2\gamma)}{2}\frac{\partial^2}{\partial z^2}+V(\rho,z)$ | $\sqrt{3}\gamma_3\left[\frac{\partial^2}{\partial\rho\partial z}+\frac{F_z-0.5+0.5B\rho^2}{\rho}\frac{\partial}{\partial z}\right]$ | $-\sqrt{3}\frac{\gamma}{2}\left[\frac{\partial^2}{\partial\rho^2}+\frac{2F_z+B\rho^2}{\rho}\frac{\partial}{\partial\rho}+\frac{F_z(F_z-1)-0.75}{\rho^2}+(F_z+0.5)B+\frac{B^2\rho^2}{4}\right]$ | 0 |
| $\sqrt{3}\gamma_3\left[\frac{\partial^2}{\partial\rho\partial z}-\frac{F_z-1.5+0.5B\rho^2}{\rho}\frac{\partial}{\partial z}\right]$ | $\frac{(\gamma_1-\gamma)}{2}\left[\frac{\partial^2}{\partial\rho^2}+\frac{1}{\rho}\frac{\partial}{\partial\rho}-\frac{(F_z-0.5+0.5B\rho^2)^2}{\rho^2}\right]+\frac{(\gamma_1+2\gamma)}{2}\frac{\partial^2}{\partial z^2}+V(\rho,z)$ | 0 | $-\sqrt{3}\frac{\gamma}{2}\left[\frac{\partial^2}{\partial\rho^2}+\frac{2(F_z+1+0.5B\rho^2)}{\rho}\frac{\partial}{\partial\rho}+\frac{F_z(F_z+1)-0.75}{\rho^2}+(F_z+1.5)B+\frac{B^2\rho^2}{4}\right]$ |
| $-\sqrt{3}\frac{\gamma}{2}\left[\frac{\partial^2}{\partial\rho^2}-\frac{2(F_z-1)+B\rho^2}{\rho}\frac{\partial}{\partial\rho}+\frac{F_z(F_z-1)-0.75}{\rho^2}+(F_z-1.5)B+\frac{B^2\rho^2}{4}\right]$ | 0 | $\frac{(\gamma_1-\gamma)}{2}\left[\frac{\partial^2}{\partial\rho^2}+\frac{1}{\rho}\frac{\partial}{\partial\rho}-\frac{(F_z+0.5+0.5B\rho^2)^2}{\rho^2}\right]+\frac{(\gamma_1+2\gamma)}{2}\frac{\partial^2}{\partial z^2}+V(\rho,z)$ | $-\sqrt{3}\gamma_3\left[\frac{\partial^2}{\partial\rho\partial z}+\frac{F_z+1.5+0.5B\rho^2}{\rho}\frac{\partial}{\partial z}\right]$ |
| 0 | $-\sqrt{3}\frac{\gamma}{2}\left[\frac{\partial^2}{\partial\rho^2}-\frac{2F_z+B\rho^2}{\rho}\frac{\partial}{\partial\rho}+\frac{F_z(F_z+1)-0.75}{\rho^2}+(F_z-0.5)B+\frac{B^2\rho^2}{4}\right]$ | $-\sqrt{3}\gamma_3\left[\frac{\partial^2}{\partial\rho\partial z}-\frac{F_z+0.5+0.5B\rho^2}{\rho}\frac{\partial}{\partial z}\right]$ | $\frac{(\gamma+\gamma_1)}{2}\left[\frac{\partial^2}{\partial\rho^2}+\frac{1}{\rho}\frac{\partial}{\partial\rho}-\frac{(F_z+1.5+0.5B\rho^2)^2}{\rho^2}\right]+\frac{(\gamma_1-2\gamma)}{2}\frac{\partial^2}{\partial z^2}+V(\rho,z)$ |

**Table 4.** Energies (meV) of the low-lying states with $F_z = \pm 0.5 \pm 1.5 \pm 2.5$ of a quantum ring in a magnetic field ($B = 5$ and 10 T) obtained for the different Hamiltonians studied.

| $\mathcal{H}_L$ | $\mathcal{H}_{av}$ | $\mathcal{H}_{gl}$ | $\mathcal{H}_{ex}$ | $\mathcal{H}_L$ | $\mathcal{H}_{av}$ | $\mathcal{H}_{gl}$ | $\mathcal{H}_{ex}$ |
|---|---|---|---|---|---|---|---|
| $F_z = -0,5$ $B = 5$ T | | | | $F_z = +0,5$ $B = 5$ T | | | |
| −51 | −55 | −54 | −55 | −42 | −53 | −53 | −53 |
| −60 | −60 | −60 | −60 | −55 | −57 | −57 | −57 |
| −62 | −66 | −66 | −67 | −58 | −61 | −59 | −60 |
| −63 | −69 | −67 | −67 | −62 | −63 | −65 | −65 |
| −66 | −72 | −71 | −71 | −66 | −67 | −65 | −65 |
| $F_z = -0,5$ $B = 10$ T | | | | $F_z = +0,5$ $B = 10$ T | | | |
| −45 | −58 | −56 | −56 | −43 | −54 | −53 | −54 |
| −58 | −64 | −64 | −64 | −57 | −57 | −57 | −57 |
| −59 | −72 | −71 | −72 | −57 | −62 | −59 | −60 |
| −64 | −75 | −71 | −72 | −63 | −65 | −65 | −67 |
| −70 | −76 | −74 | −75 | −68 | −68 | −68 | −68 |
| $F_z = -1,5$ $B = 5$ T | | | | $F_z = +1,5$ $B = 5$ T | | | |
| −54 | −52 | −51 | −52 | −47 | −49 | −50 | −49 |
| −55 | −68 | −67 | −67 | −58 | −53 | −52 | −53 |
| −61 | −68 | −67 | −68 | −60 | −54 | −55 | −54 |
| −64 | −73 | −71 | −72 | −63 | −58 | −57 | −58 |
| −65 | −75 | −74 | −75 | −66 | −60 | −61 | −60 |
| $F_z = -1,5$ $B = 10$ T | | | | $F_z = +1,5$ $B = 10$ T | | | |
| −47 | −55 | −53 | −53 | −44 | −46 | −42 | −45 |
| −58 | −74 | −72 | −72 | −55 | −48 | −50 | −50 |
| −61 | −75 | −73 | −74 | −56 | −50 | −51 | −51 |
| −63 | −77 | −75 | −76 | −62 | −55 | −53 | −54 |
| −65 | −82 | −80 | −81 | −66 | −57 | −60 | −59 |
| $F_z = -2,5$ $B = 5$ T | | | | $F_z = +2,5$ $B = 5$ T | | | |
| −57 | −59 | −58 | −58 | −52 | −47 | −45 | −46 |
| −57 | −75 | −74 | −74 | −61 | −48 | −50 | −49 |
| −61 | −76 | −74 | −75 | −62 | −51 | −50 | −50 |
| −66 | −78 | −77 | −77 | −66 | −54 | −56 | −56 |
| −67 | −83 | −82 | −83 | −71 | −58 | −57 | −57 |
| $F_z = -2,5$ $B = 10$ T | | | | $F_z = +2,5$ $B = 10$ T | | | |
| −50 | −64 | −62 | −62 | −50 | −34 | −30 | −32 |
| −58 | −84 | −81 | −82 | −60 | −37 | −40 | −38 |
| −63 | −84 | −82 | −83 | −62 | −44 | −40 | −42 |
| −63 | −88 | −88 | −88 | −67 | −46 | −50 | −48 |
| −66 | −91 | −89 | −89 | −72 | −52 | −50 | −51 |

which has the structure of the magnetic terms of $\mathcal{H}_L$. The roots of equation (13) are $x = \frac{a+b}{2} \pm \sqrt{(\frac{a-b}{2})^2 + c^2}$. Taking

$$\begin{aligned} a &= -(\gamma_1 + \gamma)B^2\rho^2/8 \\ b &= -(\gamma_1 - \gamma)B^2\rho^2/8 \\ c^2 &= 3\gamma^2 B^4\rho^4/64, \end{aligned} \tag{14}$$

which corresponds to the quadratic magnetic terms in $\mathcal{H}_L$, we get the roots $x = -(\gamma_1 \pm 2\gamma)B^2\rho^2/8$. They are equal to the diagonal quadratic terms in all of the other Hamiltonians.

Next, independently we define

$$\begin{aligned} a &= -(\gamma_1 + \gamma) F_z B/2 \\ b &= -(\gamma_1 - \gamma) F_z B/2 \\ c^2 &= 3\gamma^2 F_z^2 B^2/4 \end{aligned} \tag{15}$$

that yields the roots $x = -(\gamma_1 \pm 2\gamma) F_z B/2$. This is exactly the diagonal linear magnetic term in $\mathcal{H}_{av}$.

To check numerically the presented approximations we have performed calculations for the InAs/GaAs quantum rings obtained in [8] and studied in [7] with the 'volcano' geometry, a height of 1.6 nm, internal hole radius of 1 nm, external diameter 23 nm, a band offset of 60 meV and Luttinger parameters $\gamma_1 = 19.7$ and $\gamma = \gamma_3 = 8.4$. The energy levels of several lowest hole states for $F_z = \pm 0.5, \pm 1.5$ and $\pm 2.5$ have been calculated for the magnetic fields $B = 5$ and $B = 10$ T. The results are presented in table 4. One can see that the results obtained with $\mathcal{H}_{ex}$, $\mathcal{H}_{gl}$ and $\mathcal{H}_{av}$ are very similar (the largest difference is about 2 meV). The highest discrepancy appears for $\mathcal{H}_L$.

In conclusion, the influence of a magnetic field on the hole energy structure of zero-dimensional semiconductor systems, represented by a four-band $\boldsymbol{k} \cdot \boldsymbol{p}$ Hamiltonian, has been considered. We have shown that the effect of a magnetic field enters the $\boldsymbol{k} \cdot \boldsymbol{p}$ Hamiltonians in a way similar to the one-band effective mass equation i.e. by linear and quadratic terms. There are two linear terms: one associated with the envelope angular momentum (diagonal) and another associated with Bloch band-edge angular momentum (also diagonal in the 4-band model). The quadratic term is always diagonal. This makes the essential difference in comparison with the Luttinger approximation, in which these terms are not diagonal. We have discussed also several other approximations. Numerical analysis performed for a quantum-dot ring shows, that they lead to qualitatively similar results.

Financial support from Generalitat Valenciana CTIDIB-2002/189, UJI-Bancaixa P1-1B2002-01 and KBN-8T11B06218 is gratefully acknowledged.

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