ZnBl valence band Hamiltonian: axial and spherical approximations vs. rotation of the cristalline structure

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1 Luttinger LK and Burt-Foreman BF Hamiltonians

The BF Hamiltonian reads,

$$\mathbb{H}_{BF} = \begin{pmatrix} P' & S_- & -R & 0 \\ S_-^\dagger & P" & -C & -R \\ -R^\dagger & -C^\dagger & P"^* & -S_+^\dagger \\ 0 & -R^\dagger & -S_+ & P'^* \end{pmatrix} \tag{1}$$

where,

$$\begin{aligned}
P' &= \tfrac{1}{2}(k_x(L+M)k_x + k_y(L+M)k_y + k_z(2M)k_z) + \tfrac{i}{2}(k_x(N-N')k_y - k_y(N-N')k_x) \\
P" &= \tfrac{1}{6}(k_x(L+5M)k_x + k_y(L+5M)k_y + 2k_z(2L+M)k_z) + \tfrac{i}{6}(k_x(N-N')k_y - k_y(N-N')k_x) \\
P"^* &= \tfrac{1}{6}(k_x(L+5M)k_x + k_y(L+5M)k_y + 2k_z(2L+M)k_z) - \tfrac{i}{6}(k_x(N-N')k_y - k_y(N-N')k_x) \\
P'^* &= \tfrac{1}{2}(k_x(L+M)k_x + k_y(L+M)k_y + k_z(2M)k_z) - \tfrac{i}{2}(k_x(N-N')k_y - k_y(N-N')k_x) \\
R &= \tfrac{1}{2\sqrt{3}}[k_x(L-M)k_x - k_y(L-M)k_y - i(k_x(N+N')k_y + k_y(N+N')k_x)] \\
R^\dagger &= \tfrac{1}{2\sqrt{3}}[k_x(L-M)k_x - k_y(L-M)k_y + i(k_y(N+N')k_x + k_x(N+N')k_y)] \\
S_- &= -\tfrac{1}{\sqrt{3}}[k_- N k_z + k_z N' k_-] \\
S_-^\dagger &= -\tfrac{1}{\sqrt{3}}[k_z N k_+ + k_+ N' k_z] \\
S_+ &= -\tfrac{1}{\sqrt{3}}[k_+ N k_z + k_z N' k_+] \\
S_+^\dagger &= -\tfrac{1}{\sqrt{3}}[k_z N k_- + k_- N' k_z] \\
C &= -\tfrac{1}{3}(k_z(N-N')k_- - k_-(N-N')k_z) \\
C^\dagger &= -\tfrac{1}{3}(k_+(N-N')k_z - k_z(N-N')k_+)
\end{aligned} \tag{2}$$

with L, M, N, N' being the Stravinou-van Dalen mass parameters. By setting constants these parameters the BF Hamiltonian turns into the LK one:

$$\mathbb{H}_{LK} = -\begin{pmatrix} P+Q & -S & R & 0 \\ -S^\dagger & P-Q & 0 & R \\ R^\dagger & 0 & P-Q & S \\ 0 & R^\dagger & S^\dagger & P+Q \end{pmatrix} \tag{3}$$

with

$$\begin{aligned} P &= [\gamma_1(kx^2+ky^2+kz^2)]/2 \\ Q &= [\gamma_2(kx^2+ky^2-2kz^2)]/2 \\ R &= [-\sqrt{3}\gamma_2(kx^2-ky^2)+i\,2\sqrt{3}\gamma_3 kxky]/2 \\ S &= \gamma_3\sqrt{3}(kx-i\,ky)kz \\ S^\dagger &= \gamma_3\sqrt{3}kz(kx+i\,ky) \\ R^\dagger &= [-\sqrt{3}\gamma_2(kx^2-ky^2)-i\,2\sqrt{3}\gamma_3 kxky]/2 \\ Q^\dagger &= Q \end{aligned} \tag{4}$$

where $\gamma_1, \gamma_2, \gamma_3$ are the so-called Luttinger parameters, related to the Stravinou-van Dalen parameters L, M, N, N'. In particular, $L - M = -3\gamma_2$, $3L + M = -2\gamma_1 - 5\gamma_2$, $N - N' = 1 + \gamma_1 - 2\gamma_2 - 3\gamma_3$ and $N + N' = -3\gamma_3$.

2 Symmetry of the Luttinger LK and Burt-Foreman BF Hamiltonians

The symmetry of the LK Hamiltonian (or the BF) is cubic. However, by imposing the restriction $\gamma_2 = \gamma_3$ we turn it isotropic, i.e. spherical symmetric, as we show next. In terms of invariants[1] we can write the LK Hamiltonian as:

$$\mathbb{H}_{LK} = -\frac{1}{m_0}\left[(\gamma_1 + \frac{5}{2}\gamma_2)\frac{k^2}{2}\mathbb{I}_0 - \gamma_2 \sum_{i=x,y,z} k_i^2\,\mathbb{J}_i^2 - 2\gamma_3 \sum_{i=x,y,z}\{k_i, k_{i+1}\}\{\mathbb{J}_i, \mathbb{J}_{i+1}\}\right]. \tag{5}$$

Since

$$\begin{aligned} (\mathbf{k}\cdot\mathbf{J})^2 &= (\mathbf{k}\cdot\mathbf{J})(\mathbf{k}\cdot\mathbf{J}) = \sum_{i=x,y,z} k_i\,\mathbb{J}_i \sum_{j=x,y,z} k_j\,\mathbb{J}_j = \sum_{i=x,y,z} k_i^2\,\mathbb{J}_i^2 + \sum_{i\neq j}^{i,j=x,y,z} k_ik_j\,\mathbb{J}_i\mathbb{J}_j \\ &= \sum_{i=x,y,z} k_i^2\,\mathbb{J}_i^2 + \sum_{j<i}^{i,j=x,y,z} (k_ik_j\,\mathbb{J}_i\mathbb{J}_j + k_jk_i\,\mathbb{J}_j\mathbb{J}_i) \end{aligned} \tag{6}$$

and assuming that the magnetic field is zero (so that $k_ik_j = k_jk_i = (k_ik_j + k_jk_i)/2 = \{k_i, k_j\}$). Then,[2]

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[1] See eq. 19 in the internal repot of July 18,2014

[2] Warning: Voon[1] p.113 does not require the absence of magnetic field, as it must be.

$$
\begin{aligned}
(\mathbf{k}\cdot\mathbf{J})^2 &= \sum_{i=x,y,z} k_i^2\,\mathbb{J}_i^2 + 2\sum_{j<i}^{i,j=x,y,z}\{k_i,k_j\}\{\mathbb{J}_i,\mathbb{J}_j\} \\
&= \sum_{i=x,y,z} k_i^2\,\mathbb{J}_i^2 + 2\sum_{i=x,y,z}\{k_i,k_{i+1}\}\{\mathbb{J}_i,\mathbb{J}_{i+1}\} \qquad (7)
\end{aligned}
$$

and (in the absence of magnetic field) eq. 5 can be rewritten as:

$$
\mathbb{H}_{LK} = -\frac{1}{m_0}\left[(\gamma_1+\frac{5}{2}\gamma_2)\frac{k^2}{2}\mathbb{I}_0 - \gamma_2(\mathbf{k}\cdot\mathbf{J})^2 + 2(\gamma_2-\gamma_3)\sum_{i=x,y,z}\{k_i,k_{i+1}\}\{\mathbb{J}_i,\mathbb{J}_{i+1}\}\right]. \qquad (8)
$$

By imposing $\gamma_2 = \gamma_3$ then $\mathbb{H}_{LK}$ becomes isotropic.[3] A less restrictive approximation is the so-called axial approximation in which γ_2, γ_3 are replaced by $\bar{\gamma} = (\gamma_2+\gamma_3)/2$ in the R and $R^\dagger$ matrix elements of eq. 3 (H_{13}, H_{24}, H_{31} and H_{42}) but keeping γ_3 in the rest of matrix elements (S elements in eq. 3: H_{12}, H_{21}, H_{34} and H_{43}) and the same for γ_2: it is kept in $H_{ii}, i = 1,2,3,4$.

In terms of invariants, the axial approximation to the LK Hamiltonian reads,

$$
\begin{aligned}
\mathbb{H}_{LK} &= -\frac{1}{m_0}\Bigg[(\gamma_1+\frac{5}{2}\gamma_2)\frac{k^2}{2}\mathbb{I}_0 - \gamma_2\sum_{i=x,y,z} k_i^2\,\mathbb{J}_i^2 + (\gamma_2-\bar{\gamma})\,\frac{k_x^2-k_y^2}{2}\,(\mathbb{J}_x^2-\mathbb{J}_y^2) \\
&\quad -2\gamma_3\sum_{i=x,y,z}\{k_i,k_{i+1}\}\{\mathbb{J}_i,\mathbb{J}_{i+1}\} + 2(\gamma_3-\bar{\gamma})\{k_x,k_y\}\{\mathbb{J}_x,\mathbb{J}_y\}\Bigg]. \qquad (9)
\end{aligned}
$$

i.e., a term $-\frac{1}{m_0}\left[(\gamma_2-\bar{\gamma})\,\frac{k_x^2-k_y^2}{2}\,(\mathbb{J}_x^2-\mathbb{J}_y^2) + 2(\gamma_3-\bar{\gamma})\{k_x,k_y\}\{\mathbb{J}_x,\mathbb{J}_y\}\right]$ with $\bar{\gamma} = (\gamma_2+\gamma_3)/2$, is added to the Hamiltonian. Of course, should $\gamma_2 = \gamma_3$ then this term is zero.

If we include an axial magnetic field then only axial symmetry (C_n) is preserved. This symmetry can be additionally reduced by an external potential, as e.g. the confining potential. Should the confining potential has the triangle symmetry then, only the C_3 symmetry group survives. Since heavy hole HH and light hole LH are degenerate at the Γ point, we face a four-fold degeneration (including spin). Then, since C_3 has only three irreps, the reduction of symmetry up to C_3, originated from the confining potential, can yield symmetry-related singular physical behaviours. Since the relevant part of the multi-band Hamiltonian describing the HH and LH states is the four-bands Hamiltonian eq. 3 (or the four-bands Hamiltonian eq. 1 for position-dependent mass parameters), we restrict ourselves to the four-band Hamiltonian. The inclusion of the split-off bands yielding the six-band Hamiltonian would reflect a similar behaviour in the presence of a confining potential with triangular symmetry. All the same, since HH/LH are not degenerate with the split-off band at the Γ point, no similar singular symmetry-related behaviour is expected in the presence of a confining potential with five-fold rotational

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[3] By replacing γ_2, γ_3 by $\tilde{\gamma} = (2\gamma_2+3\gamma_3)/5$ one gets the best approximation (see e.g. Efros and Rosen [2] and Ekenberg and Altarelli[3]).

symmetry.

The C_3 character table,

C_3	E	C_3^1	C_3^2	$\varepsilon = e^{i\,\frac{2\pi}{3}}$	
A	1	1	1	z	x^2+y^2
E_+	1	ε	ε^*	$e^{i\phi} = x + i\,y$	$e^{-2i\phi} = x^2 - y^2 - 2ixy$
E_-	1	ε^*	ε	$e^{-i\phi} = x - i\,y$	$e^{2i\phi} = x^2 - y^2 + 2ixy$

allow us to determine the symmetry of the matrix elements of $\mathbb{H}_{LK}$. It is straightforward to see that P, Q, S and S^+ have the C_3 group A, A, E_- and E_+ symmetries. However, as expected, R (and $R^\dagger$) has not C_3 symmetry. However, by replacing γ_2 and γ_3 by $\bar{\gamma} = (\gamma_2 + \gamma_3)/2$, i.e. by considereing the axial approximation, then $R = -\frac{\sqrt{3}}{2}\bar{\gamma}(k_x^2 - ky^2 - 2ik_xk_y)$ has E_+ symmetry (and $R^\dagger$ has E_-). From the point of view of symmetry $\mathbb{H}_{LK}$ may be represented by:

$$\begin{bmatrix} A & E_- & E_+ & 0 \\ E_+ & A & 0 & E_+ \\ E_- & 0 & A & E_- \\ 0 & E_- & E_+ & A \end{bmatrix} \quad \text{or} \quad \begin{bmatrix} 1 & \varepsilon^* & \varepsilon & 0 \\ \varepsilon & 1 & 0 & \varepsilon \\ \varepsilon^* & 0 & 1 & \varepsilon^* \\ 0 & \varepsilon^* & \varepsilon & 1 \end{bmatrix}, \tag{10}$$

the first matrix enclosing the C_3 symmetries and the second one the phase factors (C_3^1 eigenvalues) associated to the $\mathbb{H}_{LK}$ matrix elements.

Under the restriction of axial approximation the rotational symmetry of the confining potential is preserved in the full Hamiltonian, even in the presence of magnetic field. However, magnetic field do not preserve the full symmetry of the confining potential, e.g. the mirror symmetry planes σ_i, $i = 1, 2, 3$ of the confining potential are not symmetries of the complete Hamiltonian in the presence of magnetic field.

The same symmetry considerations apply to the BF Hamiltonian. In this case, the axial approximation means replacing $L - M$ and $N + N'$ by their average in the R (and $R^\dagger$) matrix elements. We note that, in terms of Luttinger parameters $\gamma_1, \gamma_2, \gamma_3$, we have that $L - M = -6\gamma_2$ and $N + N' = -6\gamma_3$. Then, the axial approximation means the same in both Hamiltoninans, as it should be. The symmetry of the BF matrix elements $P', P", P"^*, P'^*$ is A, that of $S_\pm$ and $S_\mp^\dagger$ are $E_\pm$, and that of R and $R^\dagger$ (under the axial approximation) E_+ and E_-. Finally C and $C^\dagger$ have E_- and E_+ symmetries, respectively. Then, from the point of view of symmetry $\mathbb{H}_{BF}$ may be represented by:

$$\begin{bmatrix} A & E_- & E_+ & 0 \\ E_+ & A & E_- & E_+ \\ E_- & E_+ & A & E_- \\ 0 & E_- & E_+ & A \end{bmatrix} \quad \text{or} \quad \begin{bmatrix} 1 & \varepsilon^* & \varepsilon & 0 \\ \varepsilon & 1 & \varepsilon^* & \varepsilon \\ \varepsilon^* & \varepsilon & 1 & \varepsilon^* \\ 0 & \varepsilon^* & \varepsilon & 1 \end{bmatrix}. \tag{11}$$

The eigenfunctions of these two Hamiltonians are 4-component spinors. The components of the spinor have precise C_3 symmetry: the components are basis of different irreps of C_3 with a single repetiton. This may be understood from the well know case of axially symmetric confining potentials (C_∞ symmetry group with irreps labeled by $M = 0, 1, -1, 2, -2, 3, -3, \ldots$). In this case the symmetry of the spinor components are $M, M+1, M+2$ and $M+3$. A symmetry reduction $C_\infty \to C_3$ correlates $M = 0, 1, -1, 2, -2, 3, -3, \ldots$ with $A, E_+, E_-, A, E_-, E_+, A, E_+, E_-, \ldots$ (see e.g. reference [4]). Also, these sequences can be derived from eq. 11. Since the eigenvectors components should have precise C_3 symmetry, their possible symmetries are those conjugated to the rows of the matrix in eq. 11 i.e.,

$$\begin{bmatrix} A \\ E_+ \\ E_- \\ A \end{bmatrix} \quad \begin{bmatrix} E_- \\ A \\ E_+ \\ E_- \end{bmatrix} \quad \begin{bmatrix} E_+ \\ E_- \\ A \\ E_+ \end{bmatrix} \quad \begin{bmatrix} A \\ E_+ \\ E_- \\ A \end{bmatrix}. \tag{12}$$

3 Rotation of the internal crystalline structure

The exact (non axial nor spherical approximated) Hamiltonian with a C_3 symmetry confining potential will have C_3-related properties in a more o less extension depending on the accuracy that an axial or spherical approximation describes the system. The axial approximation involves four non-diagonal matrix elements, while the spherical approximation involves all matrix elements, including the diagonal ones. Should the spherical approximation description actually holds on a system then the C_3-related properties would be preserved after a rotation of the crystalline structure with respect to the confining potential and the magnetic field (for the kinetic energy, see eq. 8, is spherically symmetric within this approximation). In the case that the spherical approximation was too severe and only the axial approximation can properly describe the physics of a system then the C_3-related properties would be destroyed by the abovementioned rotation of the crystalline structure.[4] Finally, if γ_2 is very different from γ_3 so that even the axial approximation does not hold then no C_3-related properties will be revealed even in the case of a crystalline structure grown in the 001 direction (i.e. without rotation of the internal crystalline structure).

3.1 From [001] to [111]: the rotation matrix

The rotation matrix employed is the following:[5]

$$\mathbb{M}_{rot} = \begin{pmatrix} \frac{1}{\sqrt{6}} & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{3}} \\ -\sqrt{\frac{2}{3}} & 0 & \frac{1}{\sqrt{3}} \end{pmatrix}. \tag{13}$$

We start from the Hamiltonian in the [001] direction, eqs. 1 and 3, in terms of invariants (e.g. eq. 9 for the LK Hamiltonian) and replace k_i and $\mathbb{J}_i$ appearing in these Hamiltonian as a function of the new coordinates k_i' and

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[4] However, as shown next, rotation of the crystalline structure from the [001] direction corresponding to a non-exactly axially symmetric Hamiltonian up to the [111] direction yields a new Hamiltonian that has an exact axial symmetry.

$\mathbb{J}'_i$ according to,

$$\mathbf{k} = \mathbb{M}_{rot}\mathbf{k}' \qquad \mathbb{J} = \mathbb{M}_{rot}\mathbb{J}' \tag{14}$$

Once we reach the new matrices, the prime is removed from k_i for the sake of a better presentation.

3.2 The [111] direction: LK Hamiltonian

The LK Hamiltonian in the [111] direction reads:[5, 6, 7]

$$\mathbb{H}_{LK} = -\frac{1}{2m_0}\begin{pmatrix} P+Q & -S & R & 0 \\ -S^\dagger & P-Q & 0 & R \\ R^\dagger & 0 & P-Q & S \\ 0 & R^\dagger & S^\dagger & P+Q \end{pmatrix} \tag{15}$$

with

$$\begin{array}{lcl} P+Q & = & (\gamma_1+\gamma_3)(kx^2+ky^2)+(\gamma_1-2\gamma_3)kz^2 \\ P-Q & = & (\gamma_1-\gamma_3)(kx^2+ky^2)+(\gamma_1+2\gamma_3)kz^2 \\ R & = & -\frac{1}{\sqrt{3}}(\gamma_2+2\gamma_3)k_-^2+\frac{2\sqrt{2}}{\sqrt{3}}(\gamma_2-\gamma_3)k_+kz \\ S & = & -\frac{\sqrt{2}}{\sqrt{3}}(\gamma_2-\gamma_3)k_+^2+\frac{2}{\sqrt{3}}(2\gamma_2+\gamma_3)k_-kz \end{array} \tag{16}$$

Axial approximation ($\gamma_2 = \gamma_3$) imply now eight matrix elements instead of four as in the [001] direction. However, we do not need to impose the $\gamma_2 = \gamma_3$ restriction, as the [111] Hamiltonian displays the required symmetry. Then, In a real case, $\gamma_2 \neq \gamma_3$, [001] direction will reveal a more or less closeness to the exact symmetry while the [111] will display an exact symmetry.

Please note that if we start from the Hamiltonian $\mathbb{H}_{LK}$ within the axial approximation, eq. 9, that displays rotational symmetry around the z ([001]) axis and then we perform a rotation of this Hamiltonian up to the [111] direction, then, the resulting rotated Hamiltonian has no rotational symmetry around the new z' axis pointing the [111] direction.

3.3 The [111] direction: BF Hamiltonian

The BF Hamiltonian in the [111] direction reads:

$$\mathbb{H}_{BF} = -\frac{1}{2m_0}\begin{pmatrix} P' & -S_- & R & 0 \\ -S_-^\dagger & P\text{''} & C & R \\ R^\dagger & C^\dagger & P\text{''}^* & S_+^\dagger \\ 0 & R^\dagger & S_+ & P'^* \end{pmatrix} \tag{17}$$

where,

$$
\begin{aligned}
P' &= [k_x(\gamma_1+\gamma_3)k_x + k_y(\gamma_1+\gamma_3)k_y + k_z(\gamma_1-2\gamma_3)k_z] - i\;[k_x(\gamma_1-2\gamma_2-3\gamma_3)k_y - k_y(\gamma_1-2\gamma_2-3\gamma_3)k_x] \\
P" &= [k_x(\gamma_1-\gamma_3)k_x + k_y(\gamma_1-\gamma_3)k_y + k_z(\gamma_1+2\gamma_3)k_z] - \tfrac{i}{3}\;[k_x(\gamma_1-2\gamma_2-3\gamma_3)k_y - k_y(\gamma_1-2\gamma_2-3\gamma_3)k_x] \\
S_- &= -\tfrac{1}{\sqrt{3}}\left\{(k_-\gamma_1 k_z - k_z\gamma_1 k_-) + \sqrt{2}\,[k_x(\gamma_2-\gamma_3)k_x - k_y(\gamma_2-\gamma_3)k_y + i\,(k_x(\gamma_2-\gamma_3)k_y + k_y(\gamma_2-\gamma_3)k_x)]\right. \\
&\quad \left. -2\,[2k_-(\gamma_2+\gamma_3)k_z - k_z\gamma_3 k_-]\right\} \\
S_+ &= -\tfrac{1}{\sqrt{3}}\left\{(k_+\gamma_1 k_z - k_z\gamma_1 k_+) + \sqrt{2}\,[k_x(\gamma_2-\gamma_3)k_x - k_y(\gamma_2-\gamma_3)k_y - i\,(k_x(\gamma_2-\gamma_3)k_y + k_y(\gamma_2-\gamma_3)k_x)]\right. \\
&\quad \left. -2\,[2k_+(\gamma_2+\gamma_3)k_z - k_z\gamma_3 k_+]\right\} \\
R &= -\tfrac{1}{\sqrt{3}}\left\{k_-(\gamma_2+2\gamma_3)k_- - \sqrt{2}\,[k_z(\gamma_2-\gamma_3)k_+ + k_+(\gamma_2-\gamma_3)k_z]\right\} \\
C &= -\tfrac{2}{3}\,[k_z(\gamma_1-2\gamma_2-3\gamma_3)k_- - k_-(\gamma_1-2\gamma_2-3\gamma_3)k_z]
\end{aligned}
\tag{18}
$$

4 Rotation in the Hamiltonian

Our complete Hamiltonian reads,

$$\mathbb{H} = \mathbb{H}_{BF} + \mathbb{H}_{strain} + V_{piezo}\mathbb{I} + V_{conf}\mathbb{I} + V_F\mathbb{I} + \mathbb{H}_B \tag{19}$$

where $\mathbb{H}_{BF}$, given in eq. 1, can be expressed as a function of $k_x, k_y, k_z, \mathbb{J}_x, \mathbb{J}_y, \mathbb{J}_z$. $\mathbb{H}_{strain}$ has the same form as $\mathbb{H}_{BF}$ with the products $k_i k_j$ replaced by ϵ_{ij}. $\mathbb{H}_B$ is the magnetic terms in the Hamiltonian:

$$\mathbb{H}_B = \left(\frac{B_0^2}{8}(x^2+y^2) + \frac{B_0}{2}(xk_y - yk_x)\right)\left((\gamma_1 - \frac{5}{2}\gamma_2)\mathbb{I} + \gamma_2\mathbb{J}_z^2\right) - \kappa\mu_B B_0 \mathbb{J}_z. \tag{20}$$

V_{conf}, V_F and V_{piezo} are the confining, electric and piezoelectric potentials. The magnetic and electric field points in the grown direction as shown on the left of the figure.

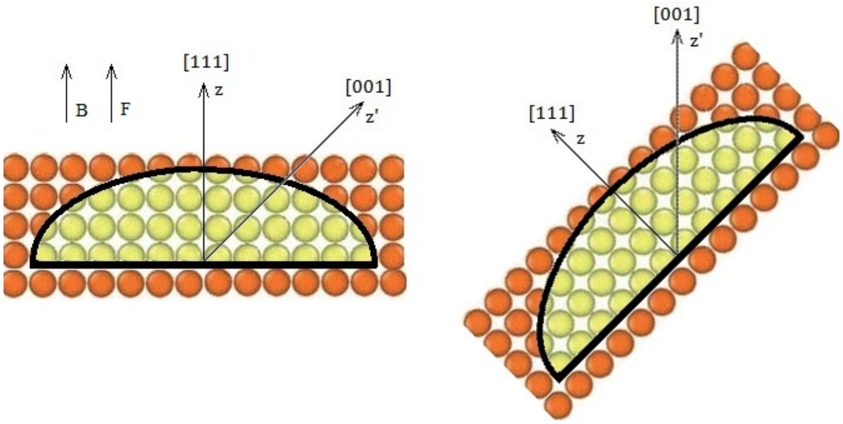

Figure 1: The system grown in [111] direction with the magnetic B and electric F fields also along this direction.

The internal crystalline structure does not grow in the standard [001] direction but in the [111] one. Then, since we have the expression of the Hamiltonian assuming the z axis to be along the [001] we must carry out some rotations. At this regards, the matrix:

$$\mathbb{M} = \begin{pmatrix} \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{6}} & -\sqrt{\frac{2}{3}} \\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} \end{pmatrix} \tag{21}$$

carry out the rotation of the coordinate axes (or the unit vectors defining them) from [001] up to [111], while its transpose (inverse) keeps the axes and carry out the rotation (transformation) of the coordinates of a vector while keeping fixed the coordinate axes (or the unit vectors defining them).

We want to keep the external axes and carry out a rotation of the crystalline structure. Then, we will use the transformation matrix $\mathbb{M}^t$ (as we alredy used it in eq. 13). On the other hand, since we only want to rotate the crystalline structure we keep unchanged the following terms of $\mathbb{H}$: $V_{conf}\mathbb{I}, V_F\mathbb{I}$ and $\mathbb{H}_B$.[5]

The matrix $\mathbb{H}_{BF}$, eq. 1, is the result of written $\mathbb{H}_{BF}$ in terms of $k_x, k_y, k_z, \mathbb{J}_x, \mathbb{J}_y, \mathbb{J}_z$ and assuming a set of axes to define the $\mathbb{J}_i$ matrices that correspond to the [001] grown. Similar considerations hold for $\mathbb{H}_{strain}$ by replacing $k_i k_j$ by ϵ_{ij}. Actually, we should write $k'_x, k'_y, k'_z, \mathbb{J}'_x, \mathbb{J}'_y, \mathbb{J}'_z$ instead, because the unprimed axes correspond to the [111] grown. Then, we should change the coordinates from primed to unprimed (we change coordinates and not the axes or unit vectors). I mean, $\mathbf{k}'$ represents the k-coordinates ($\mathbb{J}$-coordinates etc.) in the primed axes ([001]) while $\mathbf{k}$ represents the k-coordinates in the unprimed axes ([111]). $\mathbb{M}$ is the matrix that turns the primed [001] axes into the unprimed [111] ones and $\mathbb{M}^t$ the matrix that applied to the k-coordinates in terms of unprimed [111] axis unit vectors yield the k-coordinates in terms of primed [001] axis unit vectors. Then we have:

$$\begin{aligned} \mathbf{k}' &= \mathbb{M}^t \mathbf{k} \\ \mathbb{J}' &= \mathbb{M}^t \mathbb{J} \\ \epsilon'_{ij} &= \mathbb{M}^t_{ia} \mathbb{M}^t_{jb} \epsilon_{ab} \end{aligned} \tag{22}$$

so that we end up with $\mathbb{H}_{BF}$ and $\mathbb{H}_{strain}$ in terms of unprimed coordinates.

We need next to introduce calculated values of the strain ϵ_{ij} in $\mathbb{H}_{strain}$. We can calculate the strain either with the geometry with z pointing [001] (right hand side of the figure) employing the elastic constants $C^{[001]}$ or alternatively we can rotate the axes and obtain the geometry on the left hand side of the figure. In the new axes the elastic constants are $C^{[111]}$ related to $C^{[001]}$ by:

$$C^{[111]}_{ijkl} = \mathbb{M}_{ia} \mathbb{M}_{jb} \mathbb{M}_{kc} \mathbb{M}_{ld} C^{[001]}_{abcd} \tag{23}$$

The calculation yields unprimed ϵ_{ij}. Finally, I must calculate the piezoelectric potential. The situation is similar: we know the relation $p'_i = \sum_k e^{[001]}_{ijk} \epsilon'_{jk}$. However, we have calculated ϵ_{ij}. Then we must rotate the axes and obtain:

$$p_i = \sum_k e^{[111]}_{ijk} \epsilon_{jk} \tag{24}$$

with $e^{[111]}_{ijk} = \sum_{a,b,c} \mathbb{M}_{ia} \mathbb{M}_{jb} \mathbb{M}_{kc} e^{[001]}_{abc}$.

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[5] Actually, despite we keep the axes and then the Bloch functions so that nothing change, we do rotate the crystalline structure thus modifying the interaction with remote bands. It turns, in particular, into a change of the diagonal perpendicular mass coefficients, those of the term $(k_x^2 + k_y^2)$, where γ_2 is replaced by γ_3. The same replacement γ_2 by γ_3 must be done in eq. 20.

5 The full symmetry of the hole wave-function

The complete scalar wave-function of a hole is a product of Bloch times envelope components, $\Psi = \sum_i f_i\, u_i$ where u_i, f_i are Bloch and envelope components, respectively. The heavy hole HH ground state of an axially symmetric QD in the absence of external fields is two-fold degenerate. The components of the Bloch functions are eigenfunctions of the z-component of the angular momentum J_z while the envelope components are eigenfunctions of the z-component of the orbital angular momentum L_z. The complete scalar wave-function is definend by the z-component of the total angular momentum F_z. The largest f_1 component of the HH (up) ground state (labeled with $F_z = 3/2$), has an orbital quantum number $M_z = 0$ while the largest f_4 component of other degenerate HH (down) ground state (labeled with $F_z = -3/2$), has also an orbital quantum number $M_z = 0$. Schematically, we may write these eigenfunctions as:

$$\left(\begin{array}{c|c} J_z & M_z \\ \hline 3/2 & 0 \\ 1/2 & 1 \\ -1/2 & 2 \\ -3/2 & 3 \end{array}\right) \quad ; \quad \left(\begin{array}{c|c} J_z & M_z \\ \hline 3/2 & -3 \\ 1/2 & -2 \\ -1/2 & -1 \\ -3/2 & 0 \end{array}\right) \tag{25}$$

If the QD confining potential is a triangular prism, then the symmetry group of the system is not $SU2$ anymore but the double group $\bar{C}_3$ of the three-fold rotational group C_3. We enclose next its calculated character table:

$\bar{C}_3$	E	C_3^1	C_3^2	C_3^3	C_3^4	C_3^5	$e^{iM\phi}$ basis
A	1	1	1	1	1	1	$M = 0, \pm 3$
E_+	1	ϵ	ϵ^*	1	ϵ	ϵ^*	$M = 1, -2$
E_-	1	ϵ^*	ϵ	1	ϵ^*	ϵ	$M = -1, 2$
$E_{1/2}$	1	$-\epsilon^*$	ϵ	-1	ϵ^*	$-\epsilon$	$M = 1/2$
$E_{-1/2}$	1	$-\epsilon$	ϵ^*	-1	ϵ	$-\epsilon^*$	$M = -1/2$
$A_{3/2}$	1	-1	1	-1	1	-1	$M = \pm 3/2$

(26)

with $\epsilon = e^{i\,\frac{2\pi}{3}}$.

The reduction of symmetry produced by the trigonal potential, symmetry-reduces the $SU2$ labels, eq. (25), to $\bar{C}_3$ ones. These, according to the above table, must be:

$$\left(\begin{array}{c|c} Bloch & Envelope \\ \hline A_{3/2} & A \\ E_{1/2} & E_+ \\ E_{-1/2} & E_- \\ A_{3/2} & A \end{array}\right) \quad ; \quad \left(\begin{array}{c|c} Bloch & Envelope \\ \hline A_{3/2} & A \\ E_{1/2} & E_+ \\ E_{-1/2} & E_- \\ A_{3/2} & A \end{array}\right) \tag{27}$$

From the above table, the irreps product table results:

	A	E_+	E_-	$E_{1/2}$	$E_{-1/2}$	$A_{3/2}$
A	A	E_+	E_-	$E_{1/2}$	$E_{-1/2}$	$A_{3/2}$
E_+		E_-	A	$A_{3/2}$	$E_{1/2}$	$E_{-1/2}$
E_-			E_+	$E_{-1/2}$	$A_{3/2}$	$E_{1/2}$
$E_{1/2}$				E_+	A	E_-
$E_{-1/2}$					E_-	E_+
$A_{3/2}$						A

(28)

The last table allow to check that the symmetry product $f_i\, u_i$ in each row of any of the two HH ground state eigenfunctions, eq. (27), is $A_{3/2}$. This $\bar{C}_3$ label replaces the $SU2$ label F_z as the symmetry label of the complete scalar wave-function of a hole.

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[6] We adapt the Hamiltonian to the phase factors related to the Bloch functions implicit used in the text, then, although equivalent, our Hamiltonian is not exactly that reported in [5].

[7] There is a mistake in the R matrix Hamiltonian element for the [111] direction in the paper by Xia [5]. We enclose here the correct factor $2\sqrt{2}/\sqrt{3}$ in R instead of the erroneous $2\sqrt{2}/3$.