

Here we extend the formalism of inversion parity as treated in [1] to our group theory needs.

1 Motivating example: the parity of eigenstates of angular momentum

Let us denote the representations equivalent to Wigner D-matrices under proper rotations as Γ_j^W . Semiconductor point groups can typically be direct products of proper point groups with C_i or semi-direct products with C_s . In both cases, we have the notion of inversion parity—an angular momentum eigenstate can behave one of two ways under inversion ($\vec{r} \rightarrow -\vec{r}$):

1. $\hat{i}|\Psi\rangle = |\Psi\rangle$, the state is invariant under inversion. We say this state is *gerade*.
2. $\hat{i}|\Psi\rangle = -|\Psi\rangle$, the state is invariant under inversion. We say this state is *ungerade*.

Under the assumption that every improper point group can be constructed as a direct or semi-direct product of a proper point group with one of the two improper groups isomorphic to Z_2 , there always exists a parity irrep Γ_P , which is defined as

$$\chi^{(\Gamma_P)}(\text{rotation}) = 1, \chi^{(\Gamma_P)}(\text{rotoinversion}) = -1$$

Atomic band orbitals, eigenstates of angular momentum operators, are integer- l spherical harmonics in spatial representations. We know the parity of these:

$$\hat{i}Y_{lm} = (-1)^l Y_{lm}$$

Hence, the representation of a basis $|l, m\rangle, m = -l, \dots, l$ becomes

$$\Gamma_l^{\text{ang}} = \begin{cases} \Gamma_{j=l}^W & l \text{ is even} \\ \Gamma_{j=l}^W \otimes \Gamma_P & l \text{ is odd} \end{cases}$$

Or, defining direct exponentiation as $\Gamma^n \equiv \bigotimes_{i=1}^n \Gamma$, we can write this more neatly as

$$\Gamma_l^{\text{ang}} = \Gamma_{j=l}^W \otimes \Gamma_P^l$$

From standard results, we know that angular momentum coupling can be represented as a direct sum of angular representations:

$$\Gamma_l^{\text{ang}} \otimes \Gamma_{l'}^{\text{ang}} = \bigoplus_{l''=|l-l'|}^{l''=l+l'} \Gamma_{l''}^{\text{ang}}$$

We can characterise this expression for a group element g :

$$\chi^{(\Gamma_l^{\text{ang}})}(g) \chi^{(\Gamma_{l'}^{\text{ang}})}(g) = \sum_{l''=|l-l'|}^{l''=l+l'} \chi^{(\Gamma_{l''}^{\text{ang}})}(g)$$

Expanding this into a direct product of the proper representations Γ_j^W , which are always gerade, we obtain

$$\chi^{(\Gamma_l^W)}(g) \chi^{(\Gamma_{l'}^W)}(g) [\chi^{(\Gamma_P)}(g)]^{l+l'} = \sum_{l''=|l-l'|}^{l''=l+l'} \chi^{(\Gamma_{l''}^W)}(g) [\chi^{(\Gamma_P)}(g)]^{l''}$$

However, this is obviously wrong, since the left side of the equation possesses an inversion parity, but the right side doesn't. To illustrate, consider G to be a direct product of a proper point group H with the group $C_i = \hat{E}, \hat{i}$. Then each element $g \in G$ can be written as $g = (h \in H, c \in C_i)$. From the definition of the parity representation, we have

$$\chi^{(\Gamma_P)}(g = (h \in H, c \in C_i)) = \begin{cases} 1 & c = \hat{E} \\ -1 & c = \hat{i} \end{cases}$$

And, consequently

$$\chi^{(\Gamma_P)}((h \in H, c \in C_i) \cdot (\hat{E}, \hat{i})) = -\chi^{(\Gamma_P)}((h \in H, c \in C_i))$$

Consider two elements in G : a rotation g and its corresponding rotoinversion $g' = g \cdot (\hat{E}, \hat{i})$. Then find the characters of g, g' in the angular momentum coupling representation for $l + l'$ odd:

$$\begin{aligned} \chi^{(\Gamma_{\text{coupling}})}(g) &= \chi^{(\Gamma_l^W)}(g) \chi^{(\Gamma_{l'}^W)}(g) [\chi^{(\Gamma_P)}(g)]^{l+l'} \\ &= \chi^{(\Gamma_l^W)}(g) \chi^{(\Gamma_{l'}^W)}(g) \\ \chi^{(\Gamma_{\text{coupling}})}(g') &= \chi^{(\Gamma_l^W)}(g') \chi^{(\Gamma_{l'}^W)}(g') [\chi^{(\Gamma_P)}(g')]^{l+l'} \\ &= -\chi^{(\Gamma_l^W)}(g') \chi^{(\Gamma_{l'}^W)}(g') \\ \chi^{(\Gamma_{\text{coupling}})}(g') &= -\chi^{(\Gamma_{\text{coupling}})}(g) \end{aligned}$$

Applying this relation to the right sides of the coupling equation:

$$\begin{aligned} \sum_{l''=|l-l'|}^{l''=l+l'} \chi^{(\Gamma_{l''}^W)}(g') [\chi^{(\Gamma_P)}(g')]^{l''} &= - \sum_{l''=|l-l'|}^{l''=l+l'} \chi^{(\Gamma_{l''}^W)}(g) [\chi^{(\Gamma_P)}(g)]^{l''} \\ \sum_{l''=|l-l'|}^{l''=l+l'} \chi^{(\Gamma_{l''}^W)}(g') (-1)^{l''} &= - \sum_{l''=|l-l'|}^{l''=l+l'} \chi^{(\Gamma_{l''}^W)}(g) \end{aligned}$$

Since Γ_j^W is defined on proper rotations, we have $\chi^{(\Gamma_j^W)}(g) = \chi^{(\Gamma_j^W)}(g')$. Hence

$$\sum_{l''=|l-l'|}^{l''=l+l'} \chi^{(\Gamma_{l''}^W)}(g) (-1)^{l''} = - \sum_{l''=|l-l'|}^{l''=l+l'} \chi^{(\Gamma_{l''}^W)}(g)$$

This obviously isn't true for a general element g and values of l, l' , since on the left side each other term of the sum has a different sign than its corresponding term on the right side.

Possible resolution? My conjecture: the decomposition of a direct product of two angular momentum eigenstate basis representations cannot be simply equated to a direct sum of similar representations when rotoinversions are introduced, since inversion parity needs to be preserved. Therefore the terms in the sum should pick up factors of Γ_P depending on the parities of l, l' , and l'' .

$$\text{My proposed solution: } \Gamma_l^{\text{ang}} \otimes \Gamma_{l'}^{\text{ang}} = \bigoplus_{l''=|l-l'|}^{l''=l+l'} \Gamma_{l''}^{\text{ang}} \otimes [\Gamma_P]^{l+l'-l''}$$

To truly prove this proposal, the fundamental nature of angular momentum coupling must be carried out.

2 The minimal Hilbert space

2.1 Definition of minimal Hilbert Space

Consider a group G of the hamiltonian \hat{H} with irreps labelled by i : Γ_a . Each irrep has a dimensionality d_a , and hence a basis consisting of d_a basis vectors. The basis vectors of irrep Γ_a can then be labelled as $|a, m\rangle$, where $m = 1, 2 \dots d_a$. As proven by Tinkham in "Group Theory and Quantum Mechanics", p.41-2:

$$\langle a, m | a', m' \rangle = \delta_{a,a'} \delta_{m,m'}$$

Then, we shall define the *minimal Hilbert space* $\mathcal{H}_G \in \mathcal{H}_{\hat{H}}$ of G as such Hilbert space so that

1. Each irrep of G has a basis in \mathcal{H}_G
2. The choice of a basis for any irrep of G in \mathcal{H}_G is unique, where each partner basis vector is a pure vector $|a, m\rangle$ (up to a reordering of the degeneracy quantum number m).

We see that the choice of \mathcal{H}_G isn't generally unique, but all \mathcal{H}_G are bijective to each other, by the uniqueness of quantum number pair a, m .

A way to construct \mathcal{H}_G is to consider all the basis vectors $|a, m\rangle$ — \mathcal{H}_G is just the Hilbert space spanned by all the basis vectors.

We see then that the group elements of G are operators in the minimal Hilbert space \mathcal{H}_G .

From standard results we know that the basis of Γ_a consists of d_a degenerate eigenstates of \hat{H} ; there might be accidental degeneracy between bases of two distinct irreps.

2.2 Direct products of groups

Consider groups G_A, G_B , with irreps labelled as Γ_a and Γ_b respectively. Then, we can immediately write down their minimal Hilbert spaces:

\mathcal{H}_{G_A} is spanned by $\{|a, m\rangle, m = 1, 2 \dots d_a\}$; \mathcal{H}_{G_B} is spanned by $\{|b, n\rangle, n = 1, 2 \dots d_b\}$

Now, consider the direct product of these groups: $G = G_A \otimes G_B$. It is a known result that all possible direct products of irreps $\Gamma_a \otimes \Gamma_b$ form the full set of irreps of G : these can be labelled by the pair of indices a, b :

$$\Gamma_{a,b} = \Gamma_a \otimes \Gamma_b$$

This relation can be written in terms of the matrices for a general group element of G :

$$D^{(\Gamma_{a,b})}(g_a \otimes g_b) = D^{(\Gamma_a)}(g_a) \otimes D^{(\Gamma_b)}(g_b)$$

Since we can construct the full set of irreps of G , we can also write down its minimal Hilbert space; we see that each basis vector of \mathcal{H}_G will be labelled by the pair a, b to

where

$$c_{lm} = \int_{S^2} Y_l^m(\theta, \phi)^* f(\theta, \phi) dV_{S^2}$$

Hence there exists a mapping from $f : S^2 \rightarrow \mathbb{C}$ onto $\mathcal{H}_{SO(3)}$:

$$f(\theta, \phi) = \sum_{l=0}^{\infty} \sum_{m=-l}^l c_{lm} \langle \hat{\alpha} | l, m \rangle \rightarrow \sum_{l=0}^{\infty} \sum_{m=-l}^l c_{lm} |l, m\rangle_{\mathcal{H}_{SO(3)}}$$

We see that there exists a mapping between the Hilbert space of $SO(3)$ and the space of functions $f : S^2 \rightarrow \mathbb{C}$ which is bijective, continuous, and its inverse is continuous as well. Hence there exists a homeomorphism (topological isomorphism) between these two spaces. We can also identify the functions $f : S^2 \rightarrow \mathbb{C}$ as wavefunctions (omitting the r dependence). Hence $\mathcal{H}_{SO(3)}$ is homeomorphic to the space of wavefunctions on the unit sphere.

2.4 The inversion symmetry of a rotationally symmetric single particle

Consider a Hamiltonian of a single particle in the form

$$\hat{H} = \text{kinetic term} + \text{potential term} = -\frac{\hbar^2}{2m} \nabla^2 + V(\hat{r}, t)$$

Suppose this Hamiltonian possesses symmetry under 3D spatial proper rotations—that is, $SO(3)$ symmetry. The kinetic term automatically possesses this symmetry, and for the potential term to possess this symmetry we require V to be independent on θ, ϕ in spherical coordinates:

$$\hat{H}_{SO(3)} = -\frac{\hbar^2}{2m} \nabla^2 + V(\hat{r}, t)$$

where \hat{r} is the radial distance operator. Now, consider the spatial inversion operator $\hat{i} : \vec{r} \rightarrow -\vec{r}$. We see that the kinetic term is symmetric under inversion; and since inversion preserves $|\vec{r}|$, a potential term only dependent on \hat{r}, t must be symmetric under inversion. Hence, \hat{H} is symmetric under inversion.

From this we see that if the Hamiltonian of a *single particle* is symmetric under rotations, it is also symmetric under rotoinversions—hence the group of the Hamiltonian is not $SO(3)$ but $O(3)$. This is not in general true for Hamiltonians of multiple particles, even if they're non-interacting.

Now, consider the group $C_i = \{\hat{E}, \hat{i}\}$, where \hat{E} is the identity operator and \hat{i} is spatial inversion. It is trivial to show that

$$O(3) = SO(3) \otimes C_i$$

Then, as per our previous result:

$$\mathcal{H}_{O(3)} = \mathcal{H}_{SO(3)} \otimes \mathcal{H}_{C_i}$$

We already know $\mathcal{H}_{SO(3)}$. To obtain \mathcal{H}_{C_i} we consult standard tables [2, p.138] to see that C_i has two irreps, characterised by the character table

C_i	E	i
Γ_1	1	1
Γ_2	1	-1

Since both irreps are 1-dimensional, we can write down the basis vectors of \mathcal{H}_{C_i} : $|n=1\rangle, |n=2\rangle$. For later convenience, we will relabel the quantum number to have a physical meaning: $|p=1\rangle = |n=1\rangle, |p=-1\rangle = |n=2\rangle$. Here p represents the parity of the vectors, which we shall define as the eigenvalue of the inversion operator. For a state with a parity p , we have

$$\hat{i} |p\rangle = p |p\rangle$$

This gives us the shape of \mathcal{H}_{C_i} , and we can now write down the basis vectors of $\mathcal{H}_{O(3)}$. $\mathcal{H}_{O(3)}$ is spanned by vectors labelled by $|l, m, p\rangle$, where

$$l = 0, 1, \dots; m = -l, -l+1, \dots, l-1, l; p = 1 \text{ or } -1$$

Now, however, an issue arises: we have shown that $\mathcal{H}_{SO(3)}$ is homeomorphic to the space of wavefunctions on S^2 . Hence $\mathcal{H}_{O(3)}$ *cannot* be homeomorphic to this space, and is rather homeomorphic to a space of wavefunctions on $2S^2$, which represents *two* disconnected unit spheres, one labelled by $p=1$ and the other by $p=-1$. Hence, the wavefunction of a general quantum state can be expressed as

$$\langle \hat{\vec{\alpha}} | \Psi \rangle = \Psi_g(\theta, \phi) |p=1\rangle + \Psi_u(\theta, \phi) |p=-1\rangle$$

where "g" and "u" mean *gerade* and *ungerade*. *Note*: the kets on the right side of the equation no longer represent Hilbert vectors, but they label the S^2 subspace of the $2S^2$ space which their respective spatial functions act on.

The wavefunction of a basis vector $|l, m, p\rangle$ is then a spherical harmonic that has definite parity:

$$\langle \hat{\vec{\alpha}} | l, m, p \rangle = Y_l^m(\theta, \phi) |p\rangle$$

Here it is important to note that we deliberately disregard the effect of inversion on the spherical harmonic functions. Indeed, if we interpret the inversion operator as taking $\vec{r} \rightarrow -\vec{r}$, we would obtain the relation

$$\hat{i} Y_l^m(\theta, \phi) = (-1)^l Y_l^m(\theta, \phi)$$

However, the $O(3)$ group element \hat{i} doesn't act on the full minimal Hilbert space $\mathcal{H}_{O(3)}$: by construction of the group as a direct product, this operator acts solely on \mathcal{H}_{C_i} —in other words, if we write a basis Hilbert vector in $\mathcal{H}_{O(3)}$ as a direct product like so:

$$|l, m, p\rangle_{\mathcal{H}_{O(3)}} = |l, m\rangle_{\mathcal{H}_{SO(3)}} \otimes |p\rangle_{\mathcal{H}_{C_i}}$$

then the inversion operator becomes:

$$\hat{i}_{\mathcal{H}_{O(3)}} = \hat{E}_{\mathcal{H}_{SO(3)}} \otimes \hat{i}_{\mathcal{H}_{C_i}}$$

This justifies our formalism for basis wavefunctions.

One might think it is contradictive to construct eigenfunctions which are odd spherical harmonics but have even inversion parity (or vice-versa). However, this doesn't actually

affect the single-particle system at all, since as its spherically symmetric Hamiltonian can be expressed as a sum of a function of only the \hat{L} operator and a purely radial function, then quantum states differing only in parity will always be degenerate, and all physical predictions stay the same. However, there will be consequences to the parity of Hamiltonian eigenstates when we consider multi-particle systems that, for example, only enjoy the symmetries of a subgroup of $O(3)$ (or $SU(2) \otimes C_i$, as shall be discussed later). There we will see a physical consequence to having a particle transforming according to an even angular momentum but to an odd inversion parity (or vice versa).

2.5 Spin states and the $SU(2)$ group

If we consider a particle with a definite angular momentum and an uncoupled spin, its group of the Hamiltonian can be written as a direct product of the angular momentum group $O(3)$ and any symmetry group that the spin-dependent part of the Hamiltonian enjoys. However, in general spin couples with angular momentum via its intrinsic magnetic moment, which corresponds to a half-integer total angular momentum eigenstate. It can be shown that the group of the Hamiltonian of a spin-orbit coupled particle is (disregarding inversions) $SU(2)$. Then the basis vectors of $\mathcal{H}_{SU(2)}$ can be labelled by j, m analogously to l, m for the $SO(3)$ group, but j , the total angular momentum, can now be half-integer:

$$\begin{array}{c} \Gamma_0 \\ \Gamma_{1/2} \\ \Gamma_1 \\ \vdots \end{array} \left| \begin{array}{ccccc} & & |j=0, m=0\rangle & & \\ & |j=\frac{1}{3}, m=-\frac{1}{2}\rangle & & |j=\frac{1}{3}, m=\frac{1}{2}\rangle & \\ |j=1, m=-1\rangle & & |j=1, m=0\rangle & & |j=1, m=1\rangle \\ & & \vdots & & \end{array} \right.$$

Analogously to $SO(3)$, when we add rotoinversions, the group of the Hamiltonian becomes $SU(2) \otimes C_i$, and its Hilbert space basis vectors will be $|j, m, p\rangle$. Each quantum number here is a function of the eigenvalue of a specific operator:

$$\begin{aligned} \hat{J} |j, m, p\rangle &= \hbar^2 j(j+1) |j, m, p\rangle \\ \hat{J}_z |j, m, p\rangle &= \hbar m |j, m, p\rangle \\ \hat{i} |j, m, p\rangle &= p |j, m, p\rangle \end{aligned}$$

And a general quantum state has a corresponding wavefunction acting on a space topologically isomorphic to $4S^2$:

$$\begin{aligned} \langle \hat{\alpha} | \Psi \rangle &= \Psi_g^+(\theta, \phi) |\uparrow, p=1\rangle + \Psi_u^+(\theta, \phi) |\uparrow, p=-1\rangle \\ &\quad + \Psi_g^-(\theta, \phi) |\downarrow, p=1\rangle + \Psi_u^-(\theta, \phi) |\downarrow, p=-1\rangle \end{aligned}$$

Note that this formulation assumes $s = 1/2$, which isn't necessarily the case—for higher spin numbers, we would require more pure-spin eigenstates. However, the homeomorphism still holds, as decomposing j into l, s eigenstates is ambiguous.

2.6 Determining parity of total angular momentum eigenstates in proper groups

Often, it is needed to reduce J -eigenstates into groups that enable improper rotations from supergroups that do not (most generally $SU(2)$). In that case, we can determine

the parities of the eigenstates under symmetry elevation that enables improper rotations by considering their *intrinsic* spatial parities directly from their wavefunctions, and subsequently carry out the symmetry breakage as needed using standard methods. For zero-spin quantum states, we know j must be an integer, and a result analogous to $SO(3)$ follows:

$$\hat{i} |j, m\rangle \Big|_{s=0} = (-1)^j |j, m\rangle$$

For $1/2$ -spin quantum states, we utilise the explicit wavefunction form as stated by Biedenharn [3, p. 283]:

$$\hat{i} |j, m\rangle \Big|_{s=1/2} = \begin{cases} (-1)^{j-1/2} |j, m\rangle & j = l + s \\ (-1)^{j+1/2} |j, m\rangle & j = l - s \end{cases}$$

For higher-spin particles, the natural inversion parity may follow a different relation, but for treatise of electrons and electron holes these two relations suffice wholly.

2.7 Total angular coupling and parity

2.7.1 Coupling for proper rotations and naive generalisation

Suppose we have two J -eigenstates that transform as Γ_j and $\Gamma_{j'}$ respectively. Disregarding any interaction between them, the system transforms as $\Gamma_j \otimes \Gamma_{j'}$, with a $(2j+1)(2j'+1)$ degeneracy. If we include an interaction term that couples the total angular momenta of these separate states, we will be able to label the resulting Hamiltonian eigenstates by j'', m'' , and to obtain their irreps we therefore need to reduce the direct product into irreps of $SU(2)$. We can utilise a standard result (CITATION):

$$\Gamma_j \otimes \Gamma_{j'} = \bigoplus_{j''=|j-j'|}^{j+j'} \Gamma_{j''}$$

Limiting $s = 0$ or $s = 1/2$ and $j = l + s$ we can immediately write down the parities of the eigenstates:

$$\hat{i} |j, m\rangle = \begin{cases} (-1)^j |j, m\rangle & j \in \mathbb{N} \\ (-1)^{j-1/2} |j, m\rangle & j + 1/2 \in \mathbb{N} \end{cases}$$

The limitation to $j = l + s$ might seem arbitrary, but we are indeed just anticipating the simplification we will be able to do in the problem we shall apply these results to. Without this limitation, it is of course necessary to separate the cases of $j = l \pm s$ and apply a different parity property to each.

Looking at the decomposition relation, we immediately see the problem: if the group of the Hamiltonian permits rotoinversions, then the left side of the equation has a definite parity (product of the parities of j and j' , respectively), but the right side does not, as the terms in the direct sum alternate in parities, as j increments by 1. Therefore, this relation cannot hold in general, since the characters of the two sides of the equations do not match, and hence the transformation properties are ill-informed. To mitigate for this, we need to employ the machinery derived above, since a general decomposition of coupled eigenstates in an improper group may span Hilbert vectors that are not present in the minimal Hilbert space of the proper subgroup.

2.7.2 Coupling for improper rotations

Suppose we couple eigenstates with total angular momenta j, j' and parities p, p' . If we mandate there be eigenstates of $j'' = |j - j'|, |j - j'| + 1 \dots j + j' - 1, j + j'$ in the decomposition of $\Gamma_{j,p} \otimes \Gamma_{j',p'}$, then the reduction of this direct product into irreps of $SU(2) \otimes C_i$ is uniquely determined precisely by mandating that all the terms of the reduction sum have the same parity, which is necessary to make the equation hold for any general reduction:

$$\Gamma_{j,p} \otimes \Gamma_{j',p'} = \bigoplus_{j''=|j-j'|}^{j+j'} \Gamma_{j'',p \cdot p'}$$

This is the necessarily the "true" formulation of the transformation law for angular momentum coupling when inversion commutes with the Hamiltonian.

For simple Hamiltonians, this only constitutes a change of formalism. If the Hamiltonian doesn't contain the \hat{i} operator, in simple cases it is reasonable to expect $\Gamma_{j,p=1}$ and $\Gamma_{j,p=-1}$ to be accidentally degenerate. Then, this parity change can hardly be detected unless specifically probed for. Whilst it may contain predictions for selection laws for complex transitions on e.g. atomic orbitals, there is a way to test whether this formalism is correct on a simpler case—that is, by breaking the aforementioned accidental degeneracy by applying only a subgroup of $SU(2) \otimes C_i$. One of such cases can be studied in excitonic transitions in quantum dots.

2.8 Predictive power of parity quantum number inclusion—quantum dots

2.8.1 Description of the physical system

Consider a semiconductor whose valence band corresponds to a p -orbital and whose conduction band corresponds to an s -orbital. An electron ($s = 1/2$) excited to the conduction band would in $SU(2) \otimes C_i$ transform according to the $\Gamma_{1/2,1}$ irrep, in accordance with previous results. A corresponding electron hole ($s = 1/2$) undergoes spin-orbit coupling which leaves it with two possible total angular momenta, $j = 1/2$ and $j = 3/2$. The $j = 1/2$ state corresponds to the split-off band which has a lower maximum energy than the valence band populated by $j = 3/2$ holes, hence we can disregard it in the experiment outlined below. The $j = 3/2$ holes transform according to $\Gamma_{3/2,-1}$, once again in accordance with previous results.

Now, consider a quantum dot grown on this semiconductor which enjoys a C_{3v} symmetry group. This group permits both proper and improper rotations, therefore its double group (describing the symmetries of spin-orbit coupled quantum states in this quantum dot) is a subgroup of $SU(2) \otimes C_i$. If we have a free hole in this quantum dot, we see its irrep in the full rotation group undergoes reduction to two irreps of C_{3v} :

$$\Gamma_{3/2,-1} = E_{1/2} \oplus (1E_{3/2} \oplus 2E_{3/2})$$

The complex-conjugate irreps can be lumped together: $(1E_{3/2} \oplus 2E_{3/2}) \equiv E_{3/2}$. These two "physical" irreps $E_{1/2}, E_{3/2}$ then describe the two characters of holes in this quantum dot, light-like and heavy-like respectively [4]. This allows two one-electron-one-hole exciton complexes to exist, labelled by Karlsson as X_{10} and X_{01} for heavy-like

and light-like holes respectively. We can then label each exciton complex by the irrep decomposition of its symmetries, which are given by the product of the irrep of the constituent electron and hole (note that the electron irrep gets reduced to $E_{1/2}$):

$$\begin{aligned} X_{10} & : & E_{3/2} \otimes E_{1/2} = 2E \\ X_{01} & : & E_{1/2} \otimes E_{1/2} = A_1 \oplus A_2 \oplus E \\ X_{10} + X_{01} & : & A_1 \oplus A_2 \oplus 3E \end{aligned}$$

This is the result Karlsson et al obtains, and using dipole approximation, it yields 4 predicted transitions to vacuum in total.

2.8.2 Naive coupling interpretation

If we used the naive angular momentum eigenstate coupling decomposition rule which disregards parity, we would obtain a different result. The two exciton complexes X_{10} and X_{01} together constitute the coupling between a $j = 1/2$ state (electron) and $j = 3/2$ state (hole in either characteristic) yields the decomposition in $SU(2)$:

$$\Gamma_{j=3/2} \otimes \Gamma_{j=1/2} = \Gamma_{j=1} \oplus \Gamma_{j=2}$$

Naively assigning odd parity to $\Gamma_{j=1}$ and even parity to $\Gamma_{j=2}$, we would obtain the following irrep decomposition in C_{3v} of the two excitonic complexes together:

$$X_{10} + X_{01} : 2A_1 \oplus 3E$$

This predicts 5 transitions to vacuum in total, which is *not* in agreement with Karlsson et al.

2.8.3 Corrected coupling interpretation

Repeating the same interpretation of $X_{10} + X_{01}$ as angular momentum coupling, we now carry this out in the full improper rotation double group $SU(2) \otimes C_i$. The $j = 1/2$ electrons transform as $\Gamma_{1/2,1}$ and the $j = 3/2$ holes transform as $\Gamma_{3/2,-1}$. They therefore decompose as

$$\Gamma_{j=3/2,p=-1} \otimes \Gamma_{j=1/2,p=1} = \Gamma_{j=1,p=-1} \oplus \Gamma_{j=2,p=-1}$$

The $j = 2$ state is now odd, in contrast to the naive case, when it is even! Reducing this further into C_{3v} irreps:

$$X_{10} + X_{01} : A_1 \oplus A_2 \oplus 3E$$

This retrieves the result Karlsson et al arrive at.

2.8.4 Note on alternative approach

For the total angular momentum quantum number, the fact an integer value of j can have two different parities can be resolved by refusing to interpret it as a $Y_j^m(\theta, \phi)$ spherical harmonic (which it isn't), but rather keeping track of the part of j that lives in spin space. For example, consider two $s = 1/2$ particles. Together, they form a $s = 0$ singlet and $s = 1$ triplet, which under spin-orbit coupling (if we place them on a s -type orbital) can be interpreted as $j = 0$ and $j = 1$ eigenstates. The triplet,

however, was constructed from mixing three states that live entirely in spin space, with no spatial dependence, and hence an implicit even parity which should be preserved under the coupling. This approach is not sufficient in this form, however, because in spin-orbit coupling neither s nor l is preserved—hence for full treatment we would have to consider *all* possible pairs l, s for each j , their parities (dictated by l alone), and how they mix together when spin-orbit coupling is introduced! Truly, the formalism developed in this treatment is much more efficient and requires less knowledge of the underlying physics of spin-orbit coupling.

Moreover, this alternative approach cannot be used for spinless systems which enjoy $O(3)$ symmetries, where the parity problem in coupling still manifests.

2.8.5 Note on Karlsson’s data

In the paper cited, there were only 3 transitions between X_{10}, X_{01} and vacuum detected. This was attributed to symmetry elevation which, for these exciton complexes, approximated the symmetry of the quantum dot to D_{3h} , a supergroup of C_{3v} . For D_{3h} , both the naive and the corrected angular momentum coupling approach yield the same number of transitions predicted. However, the symmetry elevation isn’t precise, as it only weakens certain transition photoluminescence peaks which don’t possess all D_{3h} symmetry planes, and 2 weakened peaks would be easier to resolve than just 1. Moreover, the labelling of exciton complexes by C_{3v} irreps obtained by Karlsson still contradicts the naive approach.

References

- [1] Shiau, S.-Y., Combescot, M. (2021), Missing understanding of the phase factor between valence-electron and hole operators. SEMICONDUCTORS, Vol. **55**, No. 9, pp. 1068
- [2] Altmann, S. L., Herzig, P. (1994), *Point-Group Theory Tables*. Oxford: Clarendon Press
- [3] Biedenharn, L. C., Louck, J. D. (1981), *Angular momentum in Quantum Physics: Theory and Application*, Encyclopedia of Mathematics, vol. 8
- [4] Karlsson, K. F. *et al* (2015), Spectral signatures of high-symmetry quantum dots and effects of symmetry breaking. *New Journal of Physics*, **17** 103017