

Treatment of Hilbert spaces spanned by quantum states coupling under interaction Hamiltonians and their demand of parity quantum number in angular momentum eigenstates

Michal Horanský

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Abstract

By considering parity under spatial inversion, the group of proper rotations— $SO(3)$ for spinless particles, $SU(2)$ for particles with spin—can be shown to be insufficient to describe how eigenstates of angular momenta couple when interaction terms are introduced to the Hamiltonian. To resolve this, we first introduce the concept of minimal Hilbert spaces of groups, which we then use to show that Hamiltonian eigenstates for Hamiltonians commuting with rotoinversions cannot be fully expressed as wavefunctions on a unit sphere. By considering angular momentum eigenstates with seemingly paradoxical inversion parities, we propose a new rule for angular momentum coupling, which we then generalise to total angular momentum coupling and demonstrate it to be necessary to explain labellings of exciton complexes in a C_{3v} quantum dot.

1 Minimal Hilbert space

1.1 Definition of minimal Hilbert space of a group

Consider a group G of the Hamiltonian \hat{H} with irreps labelled by index a : 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 [1, 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 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 method to construct \mathcal{H}_G is to consider all the basis vectors $|a, m\rangle$ of the irreps Γ_a of the group— \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.

1.2 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 denote which irrep it belongs to and also by the pair m, n to denote its index among the set of degenerate partner basis vectors of that irrep:

$$\mathcal{H}_G \text{ is spanned by } \{|a, b, m, n\rangle, m = 1, 2 \dots d_a, n = 1, 2 \dots d_b\}$$

But each basis vector in \mathcal{H}_G can be decomposed into a direct product of basis vectors in $\mathcal{H}_{G_A}, \mathcal{H}_{G_B}$:

$$|a, b, m, n\rangle \rightarrow |a, m\rangle \otimes |b, n\rangle$$

And each pair of basis vectors in $\mathcal{H}_{G_A}, \mathcal{H}_{G_B}$ can be written as a basis vector in \mathcal{H}_G :

$$|a, m\rangle \otimes |b, n\rangle \rightarrow |a, b, m, n\rangle$$

Hence there exists a bijection between $\mathcal{H}_{G_A} \otimes \mathcal{H}_{G_B}$ and \mathcal{H}_G ; hence we can construct it as

$$\mathcal{H}_G = \mathcal{H}_{G_A} \otimes \mathcal{H}_{G_B}$$

1.3 Minimal Hilbert space of a quantum operator

The notion of a minimal Hilbert space can be applied to a general quantum operator \hat{P} as well. Here, the definition will be different to that of a minimal Hilbert space of a group, although an analogy can be drawn between the two cases. We shall define the minimal Hilbert space $\mathcal{H}_{\hat{P}}$ as the Hilbert space spanned by the eigenstates $|p\rangle$ of \hat{P} . An equivalent definition is the smallest Hilbert space on which \hat{P} is a well-defined operator.

If we consider \hat{P} acting on some Hilbert space \mathcal{H} , then $\mathcal{H}_{\hat{P}}$ is a subspace of \mathcal{H} , as each eigenstate $|p\rangle$ picks up a degeneracy quantum number $p_i = 1, 2 \dots d_p$, where d_p is the degeneracy of $|p\rangle$ in \mathcal{H} . Then \mathcal{H} is isomorphic to the Hilbert space spanned by $|p, p_i\rangle$.

Note that the symmetry group of an operator already comes equipped with degeneracies which stem from the dimensions of its irreps. It is a subtle but important point that the group is not only constructed from the operator, but also from some arbitrary Hilbert space equipped with that operator which determines the set of commuting symmetry operators we consider! Indeed, a different choice of this arbitrary Hilbert space would result in a different symmetry group of the same operator. This is in analogy to how a different choice of the arbitrary Hilbert space directly affects the degeneracies of the eigenstates of our operator.

1.4 Full coupling Hilbert space

In this section, we prove the following theorem:

Theorem 1 *Consider an operator $\hat{A}_{\mathcal{H}}$ acting on some Hilbert space \mathcal{H} . Consider a coupling operator $\hat{C}_{\mathcal{H}_1 \otimes \mathcal{H}_2} = \hat{A}_{\mathcal{H}_1} \otimes \hat{E}_{\mathcal{H}_2} + \hat{E}_{\mathcal{H}_1} \otimes \hat{A}_{\mathcal{H}_2} + \hat{A}_{\mathcal{H}_1 \otimes \mathcal{H}_2}^{\text{int}}$, where \hat{E} is the identity operator. Then the eigenstates of the coupling operator $|c, d\rangle$ that occur by coupling the eigenstates $|a_1\rangle, |a_2\rangle$ of \hat{A} in the Hilbert spaces $\mathcal{H}_1, \mathcal{H}_2$ respectively don't necessarily belong to $\mathcal{H}_1 \otimes \mathcal{H}_2$.*

Proof. Denote the set of integers $\{1, 2 \dots k\}$ as \mathbb{N}_k . \mathcal{H} can be spanned by eigenstates of \hat{A} , denoted $|a, b\rangle$, where b is the degeneracy label which is needed due to the fact that \mathcal{H} might be larger than the minimal Hilbert space of \hat{A} . We shall denote the degeneracy of quantum number a as $d(a)$, so that $b \in \mathbb{N}_{d(a)}$.

Now consider the group G_A of all operators \hat{P} on \mathcal{H} such that $[\hat{P}, \hat{A}] = 0$. Following standard results, each degenerate set of eigenvectors $\{|a, b\rangle, b \in \mathbb{N}_{d(a)}\}$ forms a basis to some irrep Γ_α of G_A , so that there exists a mapping $f : a \rightarrow \alpha$. If we denote the dimension of Γ_α as $\Delta(\alpha)$, from this mapping we know that $d(a) = \Delta(f(a))$. Also, we shall denote the minimal Hilbert space of G_A as \mathcal{H}_{G_A} .

Consider now the coupling operator \hat{C} acting on $\mathcal{H}_1 \otimes \mathcal{H}_2$. We denote $\hat{A}_1 = \hat{A}_{\mathcal{H}_1} \otimes \hat{E}_{\mathcal{H}_2}$ and $\hat{A}_2 = \hat{E}_{\mathcal{H}_1} \otimes \hat{A}_{\mathcal{H}_2}$, so that the coupling operator can be concisely expressed as

$$\hat{C} = \hat{A}_1 + \hat{A}_2 + \hat{A}^{\text{int}}$$

Now, if $\hat{A}^{\text{int}} = 0$, there is no coupling, in which case the eigenstates of \hat{C} are most generally $|a_1, a_2, b_1, b_2\rangle$, where b_1, b_2 together form the degeneracy label with degeneracy $d(a_1)d(a_2)$. Then the group of the coupling operator is simply $G_C = G_A \otimes G_A$. In this case, the eigenstates of \hat{C} which result from coupling of $|a_1\rangle_{\mathcal{H}_1}, |a_2\rangle_{\mathcal{H}_2}$ trivially belong to $\mathcal{H}_1 \otimes \mathcal{H}_2$.

Now suppose $\hat{A}^{\text{int}} \neq 0$. This might limit the number of operators on $\mathcal{H}_1 \otimes \mathcal{H}_2$ which commute with \hat{C} , and so G_C becomes a subgroup of $G_A \otimes G_A$. Now consider all the states in $\mathcal{H}_1 \otimes \mathcal{H}_2$ which are eigenstates of both \hat{A}_1 and \hat{A}_2 . Adding the non-zero interaction term causes *symmetry breakage*, which means the irrep product $\Gamma_{f(a_1)} \otimes \Gamma_{f(a_2)}$ might be reducible in G_C , and this set of simultaneous eigenstates of \hat{A}_1, \hat{A}_2

might be reducible into basis vectors of several different irreps of G_C which therefore correspond to different eigenstates of \hat{C} up to accidental degeneracy:

$$\begin{aligned} \Gamma_{f(a_1)} \otimes \Gamma_{f(a_2)} &= \bigoplus_{c \in X(a_1, a_2)} \Gamma_{g(c)} \\ \{|a_1, a_2, b_1, b_2\rangle, \quad b_1 \in \mathbb{N}_{d(a_1)}, \quad b_2 \in \mathbb{N}_{d(a_2)}\} &= \{|c, d\rangle, \quad c \in X(a_1, a_2), \quad d \in \mathbb{N}_{d_c(c)}\} \end{aligned}$$

where $g(c)$ is the mapping from eigenvalues of \hat{C} onto the labels of G_C irreps of which the corresponding eigenstates form basis vectors, $X(a_1, a_2)$ is the set of eigenvalues of \hat{C} which emerge during the coupling of $|a_1\rangle, |a_2\rangle$, and $d_c(c)$ is the degeneracy of $|c\rangle$. Notice that since we claim that the eigenstates $|c, d\rangle$ cannot be fully contained in $\mathcal{H}_1 \otimes \mathcal{H}_2$, this degeneracy cannot be constructed so that $|c, d\rangle$ spans $\mathcal{H}_1 \otimes \mathcal{H}_2$, but it is still required to include it in here, so that the total number of states on both sides of the equation is equal, since all the states on each side of the equation are orthogonal to each other. In other words, we require

$$\sum_{c \in X(a_1, a_2)} d_c(c) = d(a_1)d(a_2)$$

Now: suppose f is non-surjective. An example would be the angular-momentum-squared operator acting on the Hilbert space isomorphic to the space of wavefunctions on a unit sphere, which has $O(3)$ symmetry on this Hilbert space, but half of the irreps of $O(3)$ don't have a basis in this Hilbert space. As per the example, f being non-surjective implies the possibility of

$$\mathcal{H}_{G_A} \notin \mathcal{H}$$

which directly leads to

$$\mathcal{H}_{G_A \otimes G_A} \notin \mathcal{H}_1 \otimes \mathcal{H}_2$$

Since for the minimal Hilbert space of the group G_C only has the condition $\mathcal{H}_{G_C} \in \mathcal{H}_{G_A \otimes G_A}$ imposed on it, it is in general possible to have

$$\mathcal{H}_{G_C} \notin \mathcal{H}_1 \otimes \mathcal{H}_2$$

In this case there exist irreps of G_C of which the basis doesn't belong to $\mathcal{H}_1 \otimes \mathcal{H}_2$. However, there is no condition on the coupling symmetry breakage saying that $X(a_1, a_2)$ cannot contain elements c so that $\Gamma_{g(c)}$ doesn't have a basis in $\mathcal{H}_1 \otimes \mathcal{H}_2$, as will be demonstrated for angular momentum operators acting on wavefunctions on a unit sphere in 2. Therefore, in general, the coupling of $|a_1\rangle, |a_2\rangle$ may yield quantum states which do not belong to $\mathcal{H}_1 \otimes \mathcal{H}_2$, quod erat demonstrandum. The Hilbert space spanned by all quantum states obtainable from coupling for a specific interaction operator $\hat{A}_{\mathcal{H}_1 \otimes \mathcal{H}_2}^{\text{int}}$, dubbed the full coupling Hilbert space, is in general a Hilbert space containing both \mathcal{H}_{G_C} and $\mathcal{H}_1 \otimes \mathcal{H}_2$ as subspaces, and its construction is in general nontrivial.

Note. It might seem strange to say that the eigenstates of \hat{C} which acts on $\mathcal{H}_1 \otimes \mathcal{H}_2$ don't necessarily belong to $\mathcal{H}_1 \otimes \mathcal{H}_2$. However it is important to note that \hat{C} can always be constructed equivalently to act on the full Hilbert space spanned by the eigenstates which occur from coupling. This equivalence means that there will be accidental¹

¹The word "accidental" here means they transform according to different irreps, i.e. no symmetry operator transforms between states of some two subsets of the full set of degenerate states.

degeneracy between irreps of G_C if their basis vectors project onto the same vector in $\mathcal{H}_1 \otimes \mathcal{H}_2$. Indeed, this theorem is a consequence of the fact that the minimal Hilbert space of a symmetry group of an operator does not have to be a subspace of the Hilbert space we construct this group from! Coupling is an easy way of reaching these states whilst preserving the accidental degeneracy. However, the accidental degeneracy gets broken when we break the symmetry of the system, as will be demonstrated in 3.

2 Proper and improper rotation groups

2.1 The minimal Hilbert space of angular momentum eigenstates

Consider the group of 3D spatial proper rotations $SO(3)$. The irreps of this group can be labelled by l , the angular momentum quantum number, $l = 0, 1, \dots$, and $d_l = 2l + 1$. The minimal Hilbert space of $SO(3)$ is then spanned by the vectors

$$\begin{array}{c} \Gamma_0 \\ \Gamma_1 \\ \Gamma_2 \\ \vdots \end{array} \left| \begin{array}{ccccc} & & & & \\ & & & & \\ |l=2, m=-2\rangle & |l=2, m=-1\rangle & |l=2, m=0\rangle & |l=2, m=1\rangle & |l=2, m=2\rangle \\ & & \vdots & & \end{array} \right. \begin{array}{c} |l=0, m=0\rangle \\ |l=1, m=0\rangle \\ |l=1, m=1\rangle \\ |l=1, m=-1\rangle \\ |l=1, m=0\rangle \\ |l=1, m=1\rangle \\ \vdots \end{array}$$

Here we shifted the intervals of m so that they are centered about 0; this is convenient, as m now represents a real physical quantity—that is, the projection of the angular momentum onto the z -axis. This is conventional and does not affect our formalism.

Now: consider the 3D unit sphere S^2 , parametrised by $\vec{\alpha} = (\theta, \phi)$. It can be shown that there exists a mapping $\mathcal{H}_{SO(3)} \rightarrow \{f : S^2 \rightarrow \mathbb{C}\}$ such that orthogonality relations are preserved and the space of functions $f : S^2 \rightarrow \mathbb{C}$ is fully spanned by the linear combinations of vectors in $\mathcal{H}_{SO(3)}$:

$$|l, m\rangle_{\mathcal{H}_{SO(3)}} \rightarrow \langle \hat{\alpha} | l, m \rangle = Y_l^m(\theta, \phi) : S^2 \rightarrow \mathbb{C}$$

where $Y_l^m(\theta, \phi)$ are the usual spherical harmonics, normalized such that

$$\int_{S^2} Y_l^m(\theta, \phi)^* Y_{l'}^{m'}(\theta, \phi) dV_{S^2} = \delta_{l,l'} \delta_{m,m'}$$

where the integral is over the unit sphere and $dV_{S^2} = \sin \theta d\theta d\phi$ is the volume differential.

Then, as per the standard results, any function $f(\theta, \phi) : S^2 \rightarrow \mathbb{C}$ can be uniquely decomposed into spherical harmonics:

$$f(\theta, \phi) = \sum_{l=0}^{\infty} \sum_{m=-l}^l c_{lm} Y_l^m(\theta, \phi)$$

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.

2.2 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 true in general 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

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

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 state transform according to an even angular momentum but to an odd inversion parity (or vice versa).

2.3 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:

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

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.

2.4 Determining parity of total angular momentum eigenstates in proper groups

As discussed in 1.4, coupling can yield all vectors from the full coupling Hilbert space. However, for a single particle, we have not proven that it can enjoy quantum states

which do not belong to the Hilbert space equipped with its Hamiltonian. It is indeed an open question, but following intuition we assume that without coupling, only "standard" eigenstates can be reached. This assumption provides us with a tool—if we study a system of particles with coupling angular momenta, we can determine the inversion parity of each particle on its own, which gives us the parity of the coupled eigenstates of the interactive Hamiltonian. Here we outline how to find these *intrinsic* parities for some special cases within the $SU(2)$ symmetry group.

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.

2.5 Total angular momentum coupling and parity

2.5.1 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 result²:

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

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.

²This can be proven by evaluating the characters from the formula $\chi^{(\Gamma_j)}(R(\alpha)) = \sin[(j+1/2)\alpha] \sin^{-1} \alpha/2$ for any rotation by an angle α , and showing the sum holds. Since a reduction into irreps is unique by the Wonderful Orthogonality Theorem, this is sufficient proof.

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.

2.5.2 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:

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

This is 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.

3 Predictive power of parity quantum number inclusion—quantum dots

3.1 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 to 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.

3.2 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.

3.3 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.

3.4 Addenda

3.4.1 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.

3.4.2 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.

4 Summary

A Hamiltonian implies a Hilbert space which it acts on by the operators it consists of—it seems straightforward to write down their quantum numbers (or quantum number pairs, if degeneracies occur) and say the Hamiltonian is fully embedded in the Hilbert space spanned by the resulting basis vectors. However, the group of the Hamiltonian may contain irreps which don't have basis vectors in the aforementioned Hilbert space. Then if interactions occur between particles living in the system described by our Hamiltonian which couple their quantum numbers, we might by reducing the resulting representations of existing eigenstates obtain subspaces which transform according to these basis-less irreps! Therefore, we need to admit all quantum states in the Hilbert space which wholly contains not only the apparently sufficiently labelled Hamiltonian eigenstates, but also the minimal Hilbert space of the symmetry group of the Hamiltonian.

By applying this to angular momentum and total angular momentum eigenstates, we

find that they necessitate an addition of a third quantum number, the parity number p . Therefore to each state l, m two Hamiltonian eigenstate correspond: $|l, m, p = 1\rangle$ and $|l, m, p = -1\rangle$. The same principle holds for total angular momentum eigenstates labelled by j, m —the full labelling of the Hamiltonian eigenstates must be $|j, m, p\rangle$. This third quantum number is the eigenvalue of the spatial inversion operator \hat{i} . It is important to note that for $SO(3)$ the eigenstates $|l, m\rangle$ imply a parity which matches the parity of the quantum number l , however, we must admit eigenstates with the opposite parity as well. This seeming paradox is resolved by the fact that the Hilbert space spanned by these eigenstates can no longer be homeomorphically mapped onto the space of wavefunctions on the unit sphere, and thus a purely spatial representation of the eigenstates wouldn't be complete.

These additional eigenstates become important when angular momentum coupling is considered, and they make predictions for transition selection rules for exciton complexes in crystals with finite symmetry point groups.

A Appendix: The coupling of angular momenta

Here we prove that the coupling of the angular momenta of two particles preserves inversion symmetry.

The Hamiltonian of a single particle in a spherically symmetric potential can be expressed as

$$\hat{H} = \frac{1}{2m\hat{r}^2}\hat{L}^2 + \hat{H}_r$$

where $\hat{H}_r = V(\hat{r})$ is the radial dependence term and is of no interest to us, since $[\hat{r}, \hat{i}] = 0$. Also, disregarding the radial dependence, we rewrite the factor in front of \hat{L}^2 as some constant a . We have shown that $[\hat{H}, \hat{i}] = 0$, which means $[\hat{L}^2, \hat{i}] = 0$. However, we can do better than that.

Considering the angular momentum vector operator:

$$\vec{\hat{L}} = \hat{\vec{r}} \times \hat{\vec{p}}$$

we can express the angular Hamiltonian like so:

$$\hat{H}_{\text{ang}} = a\hat{L}^2 = a\vec{\hat{L}} \cdot \vec{\hat{L}}$$

We want to determine whether $\vec{\hat{L}}$ commutes with spatial inversions. To do this, we write out $\vec{\hat{p}}$ in spatial coordinates:

$$\begin{aligned}\vec{\hat{p}} &= -i\hbar\nabla \\ \vec{\hat{L}} &= -i\hbar\hat{\vec{r}} \times \nabla \\ \hat{L}_i &= -i\hbar\epsilon_{ijk}\hat{r}_j\frac{\partial}{\partial r_k}\end{aligned}$$

Hence we recover:

$$[\hat{L}_i, \hat{i}] = -i\hbar\epsilon_{ijk}[\hat{r}_j\frac{\partial}{\partial r_k}, \hat{i}]$$

Acting with this on a spatial wavefunction we obtain

$$\begin{aligned}
[\hat{L}_i, \hat{i}]f(\vec{r}) &= -i\hbar\epsilon_{ijk}[\hat{r}_j \frac{\partial}{\partial r_k}, \hat{i}]f(\vec{r}) \\
&= -i\hbar\epsilon_{ijk} \left(\hat{r}_j \frac{\partial}{\partial r_k} \hat{i}f(\vec{r}) - \hat{i} \hat{r}_j \frac{\partial}{\partial r_k} f(\vec{r}) \right) \\
&= -i\hbar\epsilon_{ijk} \left(\hat{r}_j \frac{\partial}{\partial r_k} f(-\vec{r}) - (-\hat{r}_j) \frac{\partial}{\partial r_k} f(\vec{r}) \right) \\
&= -i\hbar\epsilon_{ijk} \left(\hat{r}_j \frac{\partial(-r_k)}{\partial r_k} \frac{\partial}{\partial(-r_k)} f(-\vec{r}) - (-\hat{r}_j) \frac{\partial}{\partial r_k} f(\vec{r}) \right) \\
&= -i\hbar\epsilon_{ijk} \left(\hat{r}_j(-1) \frac{\partial}{\partial r_k} f(\vec{r}) - (-\hat{r}_j) \frac{\partial}{\partial r_k} f(\vec{r}) \right) \\
&= -i\hbar\epsilon_{ijk} \left(-\hat{r}_j \frac{\partial}{\partial r_k} f(\vec{r}) + \hat{r}_j \frac{\partial}{\partial r_k} f(\vec{r}) \right) \\
&= 0
\end{aligned}$$

Therefore

$$[\hat{\vec{L}}, \hat{i}] = 0$$

This is a strong result we can use when considering the interaction term that couples the angular momenta of two particles.

For charged particles, the coupling is caused by the interaction between their magnetic moments, which emerge from their angular momenta. The corresponding interaction term between two particles is equal to

$$\hat{H}^{\text{int}} = \xi(\hat{r}) \hat{\vec{L}}_1 \cdot \hat{\vec{L}}_2$$

We once again discard the radial dependence to write down the angular part of the full Hamiltonian for two particles:

$$\hat{H}_{\text{ang}} = a\hat{L}_1^2 + a\hat{L}_2^2 + b\hat{\vec{L}}_1 \cdot \hat{\vec{L}}_2$$

Writing this out, we can rearrange:

$$\begin{aligned}
\hat{H}_{\text{ang}} &= \hat{\vec{L}}_1 \cdot \hat{\vec{L}}_1 + \hat{\vec{L}}_2 \cdot \hat{\vec{L}}_2 + k\hat{\vec{L}}_1 \cdot \hat{\vec{L}}_2 \\
&= (\hat{\vec{L}}_1 + \hat{\vec{L}}_2) \cdot (\hat{\vec{L}}_1 + \hat{\vec{L}}_2) + (k-2)\hat{\vec{L}}_1 \cdot \hat{\vec{L}}_2
\end{aligned}$$

where $k = b/a$. We see that the dependence on \hat{L}_1^2, \hat{L}_2^2 can be rewritten as a dependence on a single operator, which we can define like so:

$$\begin{aligned}
\hat{\vec{L}}_T &= \hat{\vec{L}}_1 + \hat{\vec{L}}_2 \\
\hat{L}_T^2 &= (\hat{\vec{L}}_1 + \hat{\vec{L}}_2) \cdot (\hat{\vec{L}}_1 + \hat{\vec{L}}_2)
\end{aligned}$$

Since this operator is a function of the six angular momentum component operators of the two particles which all commute with \hat{i} , this operator also commutes with \hat{i} . Therefore, $[\hat{H}, \hat{i}] = 0$.

We can rewrite the Hamiltonian further still:

$$\hat{H}_{\text{ang}} = \frac{k}{2} \hat{L}_T^2 + \left(1 - \frac{k}{2}\right) (\hat{L}_1^2 + \hat{L}_2^2)$$

For a given pair of l_1, l_2 quantum numbers, the only free operator in this Hamiltonian is \hat{L}_T^2 , from which the labelling of the Hamiltonian eigenstates by $|l_T, m_T\rangle$ directly follows. The usual constraint $l_T = |l_1 - l_2|, |l_1 - l_2| + 1 \dots l_1 + l_2$ follows directly from the definition of $\hat{\vec{L}}_T$. Thus the Hilbert space spanned by the eigenstates of the angular momenta coupling Hamiltonian is equal to the Hilbert space spanned by the eigenstates of a single particles.

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