Quantum numbers and Angular Momentum Algebra

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Outline

- Motivation
- Discussion of single-particle and two-particle quantum numbers, uncoupled and coupled schemes
- Discussion of angular momentum recoupings and the Wigner-Eckart theorem
- Applications to specific operators like the nuclear two-body tensor force

Quantum numbers

In order to understand the basics of the nucleon-nucleon interaction and the pertaining symmetries, we need to define the relevant quantum numbers and how we build up a single-particle state and a two-body state, and obviously our final holy grail, a many-body state.

- For the single-particle states, due to the fact that we have the spin-orbit force, the quantum numbers for the projection of orbital momentum \( l \), that is \( m_l \), and for spin \( s \), that is \( m_s \), are no longer so-called good quantum numbers. The total angular momentum \( j \) and its projection \( m_j \) are then so-called good quantum numbers.

- This means that the operator \( \hat{P} \) does not commute with \( \hat{L}_x \) or \( \hat{S}_y \).

- We also start normally with single-particle state functions defined using say the harmonic oscillator. For these functions, we have no explicit dependence on \( j \). How can we introduce single-particle wave functions which have \( j \) and its projection \( m_j \) as quantum numbers?

Single-particle and two-particle quantum numbers

Motivation

When solving the Hartree-Fock project using a nucleon-nucleon interaction in an uncoupled basis (m-scheme), we found a high level of degeneracy. One sees clear from the table here that we have a degeneracy in the angular momentum \( j \), resulting in \( 2j + 1 \) states with the same energy. This reflects the rotational symmetry and spin symmetry of the nuclear forces.

<table>
<thead>
<tr>
<th>Quantum numbers</th>
<th>Energy (MeV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>( j = s )</td>
<td>-6.4022</td>
</tr>
<tr>
<td>( j = 1/2 )</td>
<td>-6.4022</td>
</tr>
<tr>
<td>( j = 3/2 )</td>
<td>-6.4026</td>
</tr>
<tr>
<td>( j = 5/2 )</td>
<td>-6.7133</td>
</tr>
<tr>
<td>( j = 7/2 )</td>
<td>-6.9403</td>
</tr>
<tr>
<td>( j = 9/2 )</td>
<td>-6.9403</td>
</tr>
<tr>
<td>( j = 11/2 )</td>
<td>-11.5886</td>
</tr>
<tr>
<td>( j = 13/2 )</td>
<td>-11.5886</td>
</tr>
<tr>
<td>( j = 15/2 )</td>
<td>-11.7201</td>
</tr>
</tbody>
</table>

Single-particle and two-particle quantum numbers, brief review on angular momenta etc

Since we have a spin orbit force which is strong, it is easy to show that the total angular momentum operator \( \hat{J} = \hat{L} + \hat{S} \) does not commute with \( \hat{L}_x \) and \( \hat{S}_y \). To see this, we calculate for example

\[
\{\hat{L}_x, \hat{J} \} = \{\hat{L}_x, \hat{L} + \hat{S}\} = \{\hat{L}_x, \hat{L}_x + \hat{S}_x + \hat{S}_y + \hat{S}_z\} = 0, \tag{1}
\]

since we have that \( \{\hat{L}_x, \hat{L}_z\} = i\hbar \hat{L}_y \) and \( \{\hat{L}_y, \hat{L}_z\} = -i\hbar \hat{L}_x \).
We have also
\[ |\hat{J}| \geq |\hat{L}| - |\hat{S}|, \]
or
\[ |\hat{J}| = \hbar \sqrt{J(J+1)} \geq |\hbar \sqrt{L(L+1)} - \hbar \sqrt{S(S+1)}|. \]

If we limit ourselves to nucleons only with \( s = \frac{1}{2} \), we find that
\[ |\hat{J}| = \hbar \sqrt{J(J+1)} \geq \hbar \sqrt{L(L+1)} - \hbar \sqrt{S(S+1)} \]
\[ \geq |\hbar \sqrt{L(L+1)} - \hbar \sqrt{S(S+1)}|. \]

It is then easy to show that for nucleons there are only two possible values of \( j \) which satisfy the inequality, namely
\[ j = l + \frac{1}{2} \text{ or } j = l - \frac{1}{2}. \]

And with \( l = 0 \) we get
\[ j = \frac{1}{2}. \]

Consider now the single-particle orbits of the 1s0d shell. For a 0d state we have the quantum numbers \( l = 2, m_l = -2, -1, 0, 1, 2 \), \( s = \frac{1}{2}, m_s = \pm \frac{1}{2}, n = 0 \) (the number of nodes of the wave function). This means that we have positive parity and
\[ j = \frac{3}{2} - l - s = m_j = \frac{3}{2}, 1, 0, 1, 2 \]
And
\[ j = \frac{5}{2} - l + s = m_j = \frac{5}{2}, 3, 4, \text{ etc...} \]
Single-particle and two-particle quantum numbers

Our single-particle wave functions, if we use the harmonic oscillator, do however not contain the quantum numbers \( j \) and \( m_j \). Normally what we have is an eigenfunction for the one-body problem defined as

\[
\psi_{\text{osc}}(r, \theta, \phi) = R_n(r) Y_{lm}^{m}(\theta, \phi),
\]

where we have used spherical coordinates (with a spherically symmetric potential) and the spherical harmonics

\[
Y_{lm}^{m}(\theta, \phi) = \frac{\sqrt{2l+1} \sqrt{4\pi}}{2^l l!} P_l^m(\cos(\theta)) \exp(i m\phi),
\]

with \( P_l^m \) being the so-called associated Legendre polynomials.

Clebsch-Gordan coefficients.

\[
\langle l_1 m_1 s_1 m_1 | l s m \rangle
\]

is a matrix element for the change of the spin-rotation algebra basis from \( l_1 m_1 s_1 m_1 \) to \( l s m \). We can thus write

\[
P_{l_1 l_2}^{l} = \sum_{m_1 m_2} Y_{l_1 m_1}^{s_1 m_1} Y_{l_2 m_2}^{s_2 m_2} \langle l_1 m_1 s_1 m_1 | l s m \rangle.
\]

Single-particle and two-particle quantum numbers

How can we get a function in terms of \( j \) and \( m_j \)? Define now

\[
\psi_{\text{osc}}(r, \theta, \phi) = R_n(r) Y_{lm}^{m}(\theta, \phi),
\]

and

\[
\psi(x, \theta, \phi),
\]

as the state with quantum numbers \( j_m \). Operating with

\[
\hat{J}^2 = (\hat{l} + \hat{s})^2 = \hat{l}^2 + \hat{s}^2 + 2 \hat{l} \cdot \hat{s},
\]

on the latter state we will obtain admixtures from possible \( \psi_{\text{osc}}(r, \theta, \phi) \) states.

Single-particle and two-particle quantum numbers

We operate with

\[
\hat{J}^2 = (\hat{l} + \hat{s})^2 = \hat{l}^2 + \hat{s}^2 + 2 \hat{l} \cdot \hat{s},
\]

on the two \( j_m \) states, that is

\[
\hat{J}^2 \psi_{\text{osc}(j=3/2, m=3/2)}^{(2m=1/2)} = \frac{3}{4} + 2m \psi_{\text{osc}(j=3/2, m=1/2)}^{(2m=1/2)},
\]

and

\[
\hat{J}^2 \psi_{\text{osc}(j=3/2, m=-1/2)}^{(2m=1/2)} = \frac{3}{4} + 2m \psi_{\text{osc}(j=3/2, m=-1/2)}^{(2m=1/2)}.
\]

Single-particle and two-particle quantum numbers

Examples are

\[
Y_{3/2} = \sqrt{\frac{3}{8\pi}},
\]

for \( l = m = 0 \),

\[
Y_{1} = \sqrt{\frac{3}{4\pi}} \cos(\theta),
\]

for \( l = 1, m = 0 \),

\[
Y_{2} = \sqrt{\frac{3}{16\pi}} (\cos^2(\theta) - 1),
\]

for \( l = 2, m = 0 \) etc.

Single-particle and two-particle quantum numbers

To see this, we consider the following example and fix

\[
\begin{aligned}
  j &= \frac{3}{2} = l - s, \\
  m_j &= \frac{3}{2}, \\
  j &= \frac{5}{2} = l + s, \\
  m_j &= \frac{3}{2},
\end{aligned}
\]

It means we can have, with \( l = 2 \) and \( s = 1/2 \) being fixed, in order to have \( m_j = 3/2 \) either \( m_l = 1 \) and \( m_s = 1/2 \) or \( m_l = -1/2 \) and \( m_s = -1/2 \). The two states

\[
\psi_{\text{osc}(j=5/2, m=3/2)}^{(2m=1/2)}
\]

and

\[
\psi_{\text{osc}(j=5/2, m=3/2)}^{(2m=-1/2)}
\]

will have admixtures from \( \psi_{\text{osc}(j=3/2, m=1)}^{(2m=1/2)} \) and \( \psi_{\text{osc}(j=3/2, m=-1)}^{(2m=-1/2)} \). How do we find these admixtures? Note that we don’t specify the values of \( m_l \) and \( m_s \) in the functions \( \psi \).

Single-particle and two-particle quantum numbers

This means that the eigenvectors \( \psi_{\text{osc}(j=2, m=1/2)} \) etc are not eigenvectors of \( \hat{J}^2 \). The above problems gives a \( 2 \times 2 \) matrix that mixes the vectors \( \psi_{\text{osc}(j=3/2, m=1/2)} \) and \( \psi_{\text{osc}(j=3/2, m=-1/2)} \) with the states

\[
\psi_{\text{osc}(j=2, m=1/2)}^{(2m=1/2)} \quad \text{and} \quad \psi_{\text{osc}(j=2, m=-1/2)}^{(2m=-1/2)}.
\]

The unknown coefficients \( \alpha \) and \( \beta \) are the eigenvectors of this matrix. That is, inserting all values of \( m_l, m_s, s \) we obtain the matrix

\[
\begin{pmatrix}
0 & 2 & \sqrt{19}/4 \\
2 & 0 & 3/2 \\
\sqrt{19}/4 & 3/2 & 0
\end{pmatrix}
\]

whose eigenvectors are the columns of

\[
\begin{pmatrix}
2/\sqrt{3} & 1/\sqrt{3} & -2/\sqrt{3}
\end{pmatrix}
\]

These numbers define the so-called Clebsch-Gordan coupling coefficients (the overlaps between the two basis sets). We can thus write
Clebsch-Gordan coefficients

The Clebsch-Gordan coefficients $\langle m_1 m_2 | J M \rangle$ have some interesting properties for us, like the following orthogonality relations

\[
\begin{align*}
\sum_{m_3} \langle m_1 m_2 | J M \rangle \langle m_3 m_3 | J M' \rangle & = \delta_{J,J'} \delta_{M,M'} \\
\sum_{m_3} \langle m_1 m_2 | J M \rangle \langle m_3 M' | J M' \rangle & = \delta_{J,J'} \delta_{M,M'} \\
\langle m_1 m_2 | J M \rangle \langle m_3 M' | J M' \rangle & = (-1)^{J_1 + J_2 + M} \langle m_1 m_2 | J M \rangle
\end{align*}
\]

and many others. The latter will turn extremely useful when we are going to define two-body states and interactions in a coupled basis.

Quantum numbers and the Schrödinger equation in relative and CM coordinates

Our two-body state can thus be written as

\[ |(j_1 j_2) J M \rangle = \sum_{m_1 m_2} \langle j_1 m_1 j_2 m_2 | J M \rangle |j_1 m_1 \rangle |j_2 m_2 \rangle. \]

Due to the coupling order of the Clebsch-Gordan coefficient it reads as $j_1$ coupled to $j_2$ to yield a final angular momentum $J$. If we invert the order of coupling we would have

\[ |(j_2 j_1) J M \rangle = \sum_{m_1 m_2} \langle j_2 m_1 j_1 m_2 | J M \rangle |j_1 m_1 \rangle |j_2 m_2 \rangle, \]

and due to the symmetry properties of the Clebsch-Gordan coefficient we have

\[ |(j_2 j_1) J M \rangle = (-1)^{J_1 + J_2 + M} \sum_{m_1 m_2} \langle j_2 m_1 j_1 m_2 | J M \rangle |j_1 m_1 \rangle |j_2 m_2 \rangle = (-1)^{J_1 + J_2} |(j_1 j_2) J M \rangle. \]

Clebsch-Gordan coefficients, testing the orthogonality relations

The orthogonality relation can be tested using the symbolic python package `wigner`. Let us test

\[ \sum_{m_1} \langle j_1 m_1 j_2 m_2 | J M \rangle \langle j_3 m_3 j_4 m_4 | J M' \rangle = \delta_{J_1 J_2} \delta_{M M'}. \]

The following program tests this relation for the case of $j_1 = 3/2$ and $j_2 = 3/2$ meaning that $m_1$ and $m_2$ run from $-3/2$ to $3/2$.

```
from sympy import S
from sympy.physics.wigner import clebsch_gordan

print(sum([clebsch_gordan(j, j, J, m, m) for j in range(-1, 1 + 1) for J in range(-2, 2 + 1) for m in range(-2, 2 + 1)]))
```

Quantum numbers and the Schrödinger equation in relative and CM coordinates

Summing up, for the single-particle case, we have the following eigenfunctions

\[ \psi_{nm_i} = \sum_{nm} \langle n m | \phi_{nm} \rangle \phi_{nm}, \]

where the coefficients $\langle n m | \phi_{nm} \rangle$ are the so-called Clebsch-Gordan coefficients. The relevant quantum numbers are $n$ (related to the principal quantum number and the number of nodes of the wave function) and

\[
\begin{align*}
\hat{J}_x \psi_{nm_i} & = m \hbar \psi_{nm_i}, \\
\hat{J}_y \psi_{nm_i} & = \hbar n \psi_{nm_i}, \\
\hat{J}_z \psi_{nm_i} & = \hbar S (S + 1) \psi_{nm_i}, \\
\hat{J}_2 \psi_{nm_i} & = \hbar^2 (J(J + 1)) \psi_{nm_i},
\end{align*}
\]

and

\begin{align*}
| (j_1 j_2) J M \rangle & = \sum_{m_1 m_2} \langle j_1 m_1 j_2 m_2 | J M \rangle |j_1 m_1 \rangle |j_2 m_2 \rangle, \\
| (j_2 j_1) J M \rangle & = (-1)^{J_1 + J_2 + M} \sum_{m_1 m_2} \langle j_2 m_1 j_1 m_2 | J M \rangle |j_1 m_1 \rangle |j_2 m_2 \rangle.
\end{align*}

Quantum numbers

We have thus the coupled basis

\[ |(j_1 j_2) J M \rangle = \sum_{m_1 m_2} \langle j_1 m_1 j_2 m_2 | J M \rangle |j_1 m_1 \rangle |j_2 m_2 \rangle, \]

and the uncoupled basis

\[ |j_1 m_1 \rangle |j_2 m_2 \rangle. \]

The latter can easily be generalized to many single-particle states whereas the first needs specific coupling coefficients and definitions of coupling orders. The m-scheme basis is easy to implement numerically and is used in most standard shell-model codes. Our coupled basis obeys also the following relations

\[
\begin{align*}
\hat{\mathcal{P}}| (j_1 j_2) J M \rangle & = \hbar^2 (J(J + 1)) |(j_1 j_2) J M \rangle, \\
\hat{\mathcal{L}}| (j_1 j_2) J M \rangle & = \hbar J |(j_1 j_2) J M \rangle, \\
\hat{\mathcal{J}}| (j_1 j_2) J M \rangle & = \hbar J |(j_1 j_2) J M \rangle.
\end{align*}
\]
The nuclear forces are almost charge independent. If we assume they are, we can introduce a new quantum number which is conserved. For nucleons only, that is a proton and neutron, we can limit ourselves to two possible values which allow us to distinguish between the two particles. If we assign an isospin value of \( T = 1/2 \) for protons and neutrons (they belong to an isospin doublet, in the same way we discussed the spin 1/2 multiplet), we can define the neutron to have isospin projection \( T_z = +1/2 \) and a proton to have \( T_z = -1/2 \). These assignments are the standard choices in low-energy nuclear physics.

We can in turn define the isospin Pauli matrices (in the same as we define the spin matrices) as

\[
\hat{\tau}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},
\]

\[
\hat{\tau}_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix},
\]

and

\[
\hat{\tau}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},
\]

and operating with \( \hat{\tau}_z \) on the proton state function we have

\[
\hat{\tau}_z \psi_p(r) = \frac{1}{2} \psi_p(r),
\]

and for neutrons we have

\[
\hat{\tau}_z \psi_n(r) = -\frac{1}{2} \psi_n(r).
\]

The isospin Hamiltonian is a scalar in isospin space.

The total isospin is defined as

\[
T = \sum_{i=1}^{A} \hat{\tau}_i,
\]

and its corresponding isospin projection as

\[
T_z = \sum_{i=1}^{A} \hat{\tau}_z,
\]

with eigenvalues \( T(T+1) \) for \( \hat{T} \) and \( 1/2(N-Z) \) for \( \hat{T}_z \), where \( N \) is the number of neutrons and \( Z \) the number of protons.

If charge is conserved, the Hamiltonian \( \hat{H} \) commutes with \( \hat{T}_z \) and all members of a given isospin multiplet (that is the same value of \( T \) ) have the same energy and there is no \( \hat{T}_z \) dependence and we say that \( \hat{H} \) is a scalar in isospin space.

The nuclear forces are almost charge independent. If we assume they are, we can introduce a new quantum number which is conserved. For nucleons only, that is a proton and neutron, we can limit ourselves to two possible values which allow us to distinguish between the two particles. If we assign an isospin value of \( T = 1/2 \) for protons and neutrons (they belong to an isospin doublet, in the same way we discussed the spin 1/2 multiplet), we can define the neutron to have isospin projection \( T_z = +1/2 \) and a proton to have \( T_z = -1/2 \). These assignments are the standard choices in low-energy nuclear physics.

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Angular momentum algebra, Wigner-Eckart theorem, Examples

For a one-hole-one-particle state we have
\[ |_{16}O_{1p1h} = (aj)M = a^\dagger j a |_{16}O \]
and finally for a two-particle-two-hole state we
\[ |_{16}O_{2p2h} = (abij)M = a^\dagger b a^\dagger j a |_{16}O \]
We can compute this matrix element using Wick’s theorem.

Angular momentum algebra, Wigner-Eckart theorem, Examples

The implementation of the Pauli principle looks different in the J-scheme compared with the m-scheme. In the latter, no two fermions or more can have the same set of quantum numbers. In the J-scheme, when we write a state with the shorthand
\[ |_{18}O_{J} = (ab)J M | \]
we do refer to the angular momenta only. This means that another way of writing the last state is
\[ |_{18}O_{J} = (Jb)JM | \]
We will use this notation throughout when we refer to a two-body state in J-scheme. The Kronecker δ function in the normalization factor refers thus to the values of \( j_b \) and \( j_s \). If two identical particles are in a state with the same \( j \)-value, then only even values of the total angular momentum apply. In the notation below, when we label a state as \( j \), it will actually represent all quantum numbers except \( m \).
Angular momentum algebra, two-body matrix elements

The two-body matrix element is a scalar and since it obeys rotational symmetry, it is diagonal in \(J\)-scheme, meaning that the corresponding matrix element in \(J\)-scheme is

\[
\langle J_a,J_b|M|J_c,J_d\rangle = N_{JM} \sum_{m_a,m_b,m_c,m_d} \langle m_a,m_b|m_J|J_c,J_d\rangle \langle m_a,m_b|m_J|J_c,J_d\rangle,
\]

and note that of the four \(m\)-values in the above sum, only three are independent due to the constraint \(m_a + m_b = M = m_c + m_d\).

The Hartree-Fock potential

We rewrite

\[
\text{Hartree-Fock potential}
\]

The Hartree-Fock potential

We can now use the above relations to compute the Hartree-Fock energy in \(J\)-scheme. In \(m\)-scheme we define the Hartree-Fock energy as

\[
\epsilon^{\text{HF}}_p = \epsilon_p + \sum_{i \leq F} \langle \phi_i|V|\phi_i\rangle_{AS},
\]

where the single-particle states \(\phi_i\) point to the quantum numbers in \(m\)-scheme. For a state with for example \(j = \frac{5}{2}\), this results in six identical values for the above potential. We would obviously like to reduce this to one only by rewriting our equations in \(J\)-scheme. Our Hartree-Fock basis is orthogonal by definition, meaning that we have

\[
\epsilon^{\text{HF}}_p = \epsilon_p + \sum_{i \leq F} \langle p|V|p\rangle_{AS}.
\]
First order in the potential energy

In a similar way it is easy to show that the potential energy contribution to the ground state energy in m-scheme

$$\frac{1}{2} \sum \langle j m_j | m_f \rangle \langle j m_j | M | \hat{V} \rangle | j m_f \rangle | M \rangle_{AS},$$

can be rewritten as

$$\frac{1}{2} \sum_{j, m} \sum_j (2J + 1) \langle j m | \hat{V} | j m \rangle | J \rangle_{AS}.$$ 

This reduces the number of floating point operations with an order of magnitude on average.

Angular momentum algebra

We define an irreducible spherical tensor $T_\lambda^\mu$ of rank $\lambda$ as an operator with $2\lambda + 1$ components $\mu$ that satisfies the commutation relations ($\hbar = 1$)

$$[J_+, T_\lambda^\mu] = \sqrt{(\lambda + \mu)(\lambda - \mu + 1)} T_\lambda^{\mu + 1},$$

and

$$[J_z, T_\lambda^\mu] = \mu T_\lambda^\mu.$$ 

Our angular momentum coupled two-body wave function obeys clearly this definition, namely

$$\langle \Psi_{ab} | \hat{V} | \Psi_{ab} \rangle = \langle \hat{V} \rangle_{AB}$$

is a tensor of rank $J$ with $M$ components. Another well-known example is given by the spherical harmonics (see examples during today’s lecture).

We are now going to define two-body and many-body states on the angular momentum coupled basis. We will also study some specific examples, like the calculation of the tensor force.

Angular momentum algebra, Wigner-Eckart theorem

We need to show that

$$\langle \Phi_J^M | \hat{V} | \Phi_J^M \rangle,$$

is independent of $M$. To show that

$$\langle \Phi_J^M | \hat{V} | \Phi_J^M \rangle,$$

is independent of $M$, we use the ladder operators for angular momentum.

Angular momentum algebra, Wigner-Eckart theorem

We wish to apply the above definitions to the computations of a matrix element

$$\langle \Phi_J^M | T_\lambda^\mu | \Phi_J^M \rangle,$$

where we have skipped a reference to specific single-particle states. This is the expectation value for two specific states, labelled by angular momenta $J$ and $M$. These states form an orthonormal basis. Using the properties of the Clebsch-Gordan coefficients we can write

$$T_\lambda^\mu (\Phi_J^M) = \sum_{J'M' M''} \langle \lambda \mu | J' M' M'' | \lambda \mu \rangle T_\lambda^{J'} | \Phi_{J'}^{M'} \rangle | M'' \rangle,$$

and assuming that states with different $J$ and $M$ are orthonormal we arrive at

$$\langle \Phi_J^M | T_\lambda^\mu | \Phi_J^M \rangle = \langle \lambda \mu | \hat{V} | \lambda \mu \rangle (\Phi_J^M | \Phi_J^M \rangle.$$
Angular momentum algebra, Wigner-Eckart theorem

We have that
\[
\langle \Phi J M | T λ \mu | \Phi J' M' \rangle = \frac{(-1)^{J-M}}{\sqrt{2J+1}} \langle \hat{J} \Phi J M | T λ \mu | \Phi J' M' \rangle,
\]
with \((-1)^{p} = 1\) when the columns \(a, b, c\) are even permutations of the columns \(1, 2, 3\), \(p = j_a + j_b + j_c\) when the columns \(a, b, c\) are odd permutations of the columns \(1, 2, 3\), and \(p = j_a + j_b + j_c\) when all the magnetic quantum numbers \(m_i\) change sign. Their orthogonality is given by
\[
\sum_{m_1} (-j_1 m_1, m_2, m_3) - (-j'_1 m_1, m_2, m_3) = \delta_{j_1 m_1, j'_1 m_1},
\]
and
\[
\sum_{m_1} (-j_1 m_1, m_2, m_3) - (-j'_1 m_1, m_2, m_3) = \frac{1}{(2j_1 + 1)} \delta_{j_1 m_1}.
\]

Angular momentum algebra, Wigner-Eckart theorem

Using \(3j\) symbols we rewrote the Wigner-Eckart theorem as
\[
\langle \Phi J M | T λ \mu | \Phi J' M' \rangle = (-1)^{J-M} \langle \hat{J} \Phi J M | T λ \mu | \Phi J' M' \rangle.
\]

Angular momentum algebra, Wigner-Eckart theorem

For later use, the following special cases for the Clebsch-Gordan and \(3j\) symbols are rather useful
\[
\langle JM J M'(00) \rangle = \frac{(-1)^{J-M}}{\sqrt{2J+1}} \langle \hat{J} 0 0 | J M M' \rangle,
\]
and
\[
\langle J k l M M' \rangle = (-1)^{J-M} \frac{M}{\sqrt{(2J+1)(J+1)}} \langle J M M' \rangle.
\]

Angular momentum algebra, Wigner-Eckart theorem

This relation can in turn be used to compute the expectation value of some simple reduced matrix elements like
\[
\langle \Phi J M | T λ \mu | \Phi J' M' \rangle = \sum_{M M'} (-1)^{J-M} \langle \hat{J} M M' | T λ \mu | \Phi J' M' \rangle,
\]
where we used
\[
\langle JM J M'(00) \rangle = \frac{(-1)^{J-M}}{\sqrt{2J+1}} \langle \hat{J} 0 0 | J M M' \rangle.
\]
Similar to the hermitian adjoint of the operator $T^l_j$, we see via the commutation relations that $(T^l_j)^\dagger$ is not an irreducible tensor, that is

$$[J_M, (T^l_j)^\dagger] = -\sqrt{(\lambda + \mu)(\lambda + \mu + 1)}(T^l_{\lambda + \mu + 1})^\dagger,$$

and

$$[J_M, (T^l_j)^\dagger] = -\mu (T^l_j)^\dagger.$$

The hermitian adjoint $(T^l_j)^\dagger$ is not an irreducible tensor. As an example, consider the spherical harmonics for $l = 1$ and $m = \pm 1$. These functions are

$$V^{1,\pm 1}_{\pm 1} (\theta, \phi) = -\sqrt{\frac{3}{4\pi}} \sin (\theta) \exp (\pm i\phi),$$

and

$$V^{1,\pm 1}_{\pm 1} (\theta, \phi) = \sqrt{\frac{3}{8\pi}} \sin (\theta) \exp (\mp i\phi).$$

With the modified quantity $T^l_j = (-1)^{l+\mu} (T^l_j)^\dagger$, we can then define the expectation value

$$\langle \Phi^l_j | T^l_j | \Phi^l_{j'} \rangle = \langle \lambda \mu | J M \rangle \langle J^l | \Phi^l_j \rangle \langle \Phi^l_j | T^l_j | \Phi^l_{j'} \rangle,$$

where the Clebsch-Gordan coefficients are real. The rhs is equivalent with

$$\langle \lambda \mu | J M \rangle | \Phi^l_j \rangle \langle \Phi^l_j | T^l_j | \Phi^l_{j'} \rangle = \langle \Phi^l_j | (T^l_j)^\dagger | \Phi^l_{j'} \rangle,$$

which is equal to

$$\langle \Phi^l_j | (T^l_j)^\dagger | \Phi^l_{j'} \rangle = (-1)^{1+\nu} (\lambda - \mu | J M | \langle \Phi^l_j | T^l_j | \Phi^l_{j'} \rangle).$$

Let us now apply the theorem to some selected expectation values. In several of the expectation values we will meet when evaluating explicit matrix elements, we will have to deal with expectation values involving spherical harmonics. A general central interaction can be expanded in a complete set of functions like the Legendre polynomials, that is, we have an interaction, with $v = |r_i - r_j|$, $v \left( \theta_0 \right) = \sum_{\mu \nu} v_{\mu \nu} (\theta_0) P_\mu (\cos \theta_0),$

with $P_\mu$ being Legendre polynomials.

$$P_\mu (\cos \theta_0) = \sum_{\mu} \frac{4\pi}{2\mu + 1} \, Y^\mu_{\mu} \left( \Omega_{\theta_0} \right).$$

We will come back later to how we split the above into a contribution that involves only one of the coordinates.

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Angular momentum algebra, Wigner-Eckart theorem

This means that we will need matrix elements of the type

\[ \langle \ell' | \ell \rangle = \sum_{m' m} | \ell m | \ell' m' \rangle 

We can rewrite the Wigner-Eckart theorem as

\[ \langle \ell' | \ell \rangle = \sum_{m' m} | \ell m | \ell' m' \rangle Y_{\ell m}^{\ast} Y_{\ell' m'} \]

This equation is true for all values of \( \theta \) and \( \phi \). It must also hold for \( \theta = 0 \).

Angular momentum algebra, Wigner-Eckart theorem

Till now we have mainly been concerned with the coupling of two angular momenta \( j_a \) and \( j_b \) to a final angular momentum \( J \). If we wish to describe a three-body state with a final angular momentum \( J \), we need to couple three angular momenta, say the two momenta \( j_a, j_b \) to a third one \( j_c \). The coupling order is important and leads to a loss trivial implementation of the Pauli principle. We can combine the angular momenta in \( m \)-scheme a three-body Slater determinant is represented as (say for the case of \( ^{16}O \), three neutrons outside the core of \( ^{16}O \)),

\[ |^{16}O \rangle = |abc \rangle |M \rangle = | \sum_{m_{abc}} \langle m_{abc} | abc \rangle | m_{abc} \rangle |M \rangle = | \Phi \rangle \]

The Pauli principle is automatically implemented via the anti-commutation relations.

Angular momentum algebra, Wigner-Eckart theorem

Now, nothing hinders us from recoupling this state by coupling \( j_b \) to \( j_c \) to yield an intermediate angular momentum \( J_{ab} \), then to \( j_a \) yielding the final angular momentum \( J \).

That is, we can have

\[ | j_a \rangle | j_b \rangle | j_c \rangle |M \rangle = \sum_{m_{abc}} | j_a m_{abc} | j_b m_{abc} | j_c M_{abc} \rangle |M \rangle \]

We will always assume that we work with orthonormal states, this means that when we compute the overlap between these two possible ways of coupling angular momenta, we get

\[ \langle j_a | j_c \rangle | j_b \rangle | M' \rangle | j_a \rangle | j_b \rangle | j_c \rangle |M \rangle = \delta_{j_a j_c} \delta_{M' M} \sum_{m_{abc}} | j_a m_{abc} \rangle \langle j_a m_{abc} | j_c M_{abc} \rangle \]

We have

\[ \langle Y_{\ell'} | Y_{\ell} \rangle = \sum_{m' m} | \ell m | \ell' m' \rangle Y_{\ell m}^{\ast} Y_{\ell' m'} \]

and for \( \theta = 0 \), the spherical harmonic

\[ Y_{\ell m}(\theta = 0, \phi) = \sqrt{\frac{2\ell + 1}{4\pi}} \delta_{m 0} \]

which results in

\[ \langle Y_{\ell'} | Y_{\ell} \rangle = \left( \frac{2\ell + 1}{4\pi} \right)^{1/2} \delta_{\ell \ell'} \delta_{m m'} \]

Angular momentum algebra, Wigner-Eckart theorem

However, when we deal the same state in an angular momentum coupled basis, we need to be a little bit more careful. We can namely couple the states as follows:

\[ | j_b \rangle | j_a \rangle | j_c \rangle |M \rangle = \sum_{m_{abc}} | j_a m_{abc} | j_b m_{abc} | j_c M_{abc} \rangle |M \rangle \]

that is, we couple first \( j_a \) to \( j_b \) to yield an intermediate angular momentum \( J_{ab} \), then to \( j_c \) yielding the final angular momentum \( J \).

We use then the latter equation to define the so-called \( 6j \)-symbols

\[ \langle j_a \rangle | j_c \rangle | j_b \rangle | J' \rangle | j_a \rangle | j_b \rangle | j_c \rangle | M \rangle = \delta_{j_a j_c} \delta_{J' J} \sum_{m_{abc}} | j_a m_{abc} \rangle \langle j_a m_{abc} | j_c M_{abc} \rangle \]

where the symbol in curly brackets is the \( 6j \) symbol. A specific coupling order has to be respected in the symbol, that is, the so-called triangular relations between three angular momenta needs to be respected, that is

\[ \{ x \ x \} \{ x \ x \} \{ x \ x \} \{ x \ x \} \{ x \ x \} \{ x \ x \} \{ x \ x \} \{ x \ x \} \]

Angular momentum algebra, Wigner-Eckart theorem
Angular momentum algebra, Wigner-Eckart theorem

The $6j$ symbol is invariant under the permutation of any two columns
\[
\{ j_1 j_2 j_3 \} \rightarrow \{ j_1 j_3 j_2 \}
\]
The $6j$ symbol is also invariant if upper and lower arguments are interchanged in any two columns
\[
\{ j_1 j_2 j_3 \} \rightarrow \{ j_3 j_2 j_1 \}
\]

The $6j$ symbols satisfy this orthogonality relation
\[
\sum_{j_3} (2j_3 + 1) \delta_{j_1 j_2 + j_3}^{j_4 j_5 j_6} = \frac{(-1)^{j_1+j_2+j_4}}{(2j_1 + 1)(2j_2 + 1)}
\]
The symbol $(j_1j_2j_3)$ (called the triangular delta) is equal to one if the triad $(j_1j_2j_3)$ satisfies the triangular conditions and zero otherwise. A useful value is given when say one of the angular momenta are zero, say $j_6 = 0$, then we have
\[
\{ j_1 j_2 j_3 \} = \left\{ \frac{(-1)^{j_1+j_2}}{(2j_1 + 1)} \right\}
\]

Testing properties of $6j$ symbols

The above properties of $6j$ symbols can again be tested using the symbolic python package wigner. Let us test the invariance
\[
\{ j_1 j_2 j_3 \} \rightarrow \{ j_1 j_3 j_2 \}
\]
The following program tests this relation for the case of $j_1 = 3/2, j_2 = 3/2, j_3 = 1/2, j_4 = 1/2, j_5 = 1/
\]

Angular momentum algebra, Wigner-Eckart theorem

With the $6j$ symbol defined, we can go back and rewrite the overlap between the two ways of recoupling angular momenta in terms of the $6j$ symbol. That is, we have
\[
|a \rightarrow [j_1 \rightarrow j_2]_a \rangle = \sum_{j_3} \left\{ j_1 j_2 j_3 \right\} \left\{ j_3 j_4 j_5 \right\} \delta_{j_1, j_2, j_3, j_4, j_5}^{j_6}
\]
Can you find the inverse relation? These relations can in turn be used to write out the fully anti-symmetrized three-body wave function in a $J$-scheme coupled basis. If you opt then for a specific coupling order, say $|a \rightarrow j_6 \rangle \rightarrow j_6 \rangle$, you need to express this representation in terms of the other coupling possibilities.

Angular momentum algebra, Wigner-Eckart theorem

Note that the two-body intermediate state is assumed to be antisymmetric but not normalized, that is, the state which involves the quantum numbers $j_a$ and $j_b$. Assume that the intermediate two-body state is antisymmetric. With this coupling order, we can rewrite (in a schematic way) the general three-particle Slater determinant as
\[
\Phi(a, b, c) = A \left| \{ j_a \rightarrow j_b \}_{J} \right| \left| j_c \right|
\]
with an implicit sum over $J_a$. The antisymmetrization operator $A$ is used here to indicate that we need to antisymmetrize the state. Challenge: Use the definition of the $6j$ symbol and find an explicit expression for the above three-body state using the coupling order $|\{ j_a \rightarrow j_b \}_{J} \rangle \rightarrow j_c \rangle$.

Angular momentum algebra, Wigner-Eckart theorem

We can also coupled together four angular momenta. Consider two four-body states, with single-particle angular momenta $j_a, j_b, j_c$, and $j_d$ we can have a state with final $J$
\[
|\Phi(a, b, c, d)\rangle = \left| \{ j_a \rightarrow j_d \}_{J} \right| \left| \{ j_c \rightarrow j_d \}_{J} \right| \langle j_a \rightarrow j_d | J_a \rangle \langle j_c \rightarrow j_d | J_c \rangle
\]
where we read the coupling order as $j_d$ couples with $j_a$ given and intermediate angular momentum $J_a$. Moreover, $j_d$ couples with $j_c$ to given and intermediate angular momentum $J_d$. The two intermediate angular momenta $J_a$ and $J_d$ are in turn coupled to a final $J$. These operations involved three Clebsch-Gordan coefficients.
Alternatively, we could couple in the following order
\[
|\Phi(a, b, c, d)\rangle = \left| \{ j_a \rightarrow j_d \}_{J} \right| \left| \{ j_c \rightarrow j_d \}_{J} \right| \langle j_a \rightarrow j_d | J_a \rangle \langle j_c \rightarrow j_d | J_c \rangle
\]
The overlap between these two states
\[ \langle \{ j_a \to j_c \} J_{ac} \times \{ j_b \to j_d \} J_{bd} \rangle \]
is equal to
\[ \sum_{m_{M}} \langle m_{a} m_{b} m_{c} m_{d} m_{M} \rangle \langle j_{a} j_{b} m_{a} m_{b} \rangle \langle j_{c} j_{d} m_{c} m_{d} \rangle \langle j_{a} J_{ac} m_{M} \rangle \langle j_{b} J_{bd} M_{M} \rangle \]
\[ \times \langle j_{a} J_{ac} m_{M} \rangle \langle j_{b} J_{bd} M_{M} \rangle \langle j_{c} j_{d} m_{c} m_{d} \rangle \langle j_{a} J_{ac} m_{M} \rangle \langle j_{b} J_{bd} M_{M} \rangle \langle j_{c} j_{d} m_{c} m_{d} \rangle \langle j_{a} J_{ac} m_{M} \rangle \langle j_{b} J_{bd} M_{M} \rangle \]
\[ \times \langle j_{a} J_{ac} m_{M} \rangle \langle j_{b} J_{bd} M_{M} \rangle \langle j_{c} j_{d} m_{c} m_{d} \rangle \langle j_{a} J_{ac} m_{M} \rangle \langle j_{b} J_{bd} M_{M} \rangle \langle j_{c} j_{d} m_{c} m_{d} \rangle \langle j_{a} J_{ac} m_{M} \rangle \langle j_{b} J_{bd} M_{M} \rangle \]
with the symbol in curly brackets \( \{ \) being the 9j symbol. We see that a 6j symbol involves four Clebsch-Gordan coefficients, while the 9j symbol involves six.

A 9j symbol is invariant under reflection in either diagonal
\[ \{ j_1 j_2 j_3 \} \to \{ j_3 j_2 j_1 \} \]
\[ \{ j_4 j_5 j_6 \} \to \{ j_6 j_5 j_4 \} \]
The permutation of any two rows or any two columns yields a phase factor \((-1)^S\), where
\[ S = \sum_{i=1}^{9} j_i. \]
As an example we have
\[ \{ j_1 j_2 j_3 \} = (-1)^3 \{ j_3 j_2 j_1 \} \]
and it is zero for the \( 1S_0 \) wave.
How do we get here?

To derive the expectation value of the nuclear tensor force, we recall that the product of two irreducible tensor operators is
\[ W_{ac}^{m_{ac}} = \sum_{m_{M}} \langle m_{a} m_{b} m_{c} m_{d} m_{M} \rangle T_{ac}^{m_{M}} U_{bc}^{m_{ac}} \]
and using the orthogonality properties of the Clebsch-Gordan coefficients we can rewrite the above as
\[ T_{ac}^{m_{M}} U_{bc}^{m_{ac}} = \sum_{m_{ac}} \langle m_{a} m_{b} m_{c} m_{d} m_{M} \rangle W_{ac}^{m_{ac}}. \]
Assume now that the operators \( T \) and \( U \) act on different parts of say a wave function. The operator \( T \) could act on the spatial part only while the operator \( U \) acts only on the spin part. This means also that these operators commute. The reduced matrix element of this operator is thus, using the Wigner-Eckart theorem,
\[ \langle \{ j_a \to j_c \} W^{T} \{ j_a \to j_c \} \rangle = \sum_{m_{ac}} (-1)^{S-M} \left( J_{ac} \begin{array}{c} J_{ac} \n M \n M \end{array} \right) \]
\[ \times \langle \{ j_a \to j_c \} W^{T} \{ j_a \to j_c \} \rangle. \]
Angular momentum algebra, Wigner-Eckart theorem

Combining the last two equations from the previous slide and applying the Wigner-Eckart theorem, we arrive at (rearranging phase factors)

\[
\langle (\mu_4 \lambda_4 \mu) || W^* || (\lambda_4 \mu) \rangle = \sqrt{(2J + 1)(2r + 1)(2J' + 1)} \sum_{s, S, M} (-1)^J \langle \mu_4 || T_p || \lambda_4 \rangle \langle \mu || U_p || \lambda \rangle
\]

which can be rewritten in terms of a 9j symbol as

\[
\langle (\mu_4 \lambda_4 || W^* || (\lambda_4 \mu) \rangle = \sqrt{(2J + 1)(2r + 1)(2J' + 1)} \sum_{s, S, M} (-1)^J \langle \mu_4 || T_p || \lambda_4 \rangle \langle \mu || U_p || \lambda \rangle
\]

Angular momentum algebra, Wigner-Eckart theorem

From this expression we can in turn compute for example the spin-spin operator of the tensor force. In case \( r = 0 \), that is we two tensor operators coupled to a scalar, we can use (with \( p = q \))

\[
\langle (\mu_4 \lambda_4 || W^* || (\lambda_4 \mu) \rangle = \frac{\delta_{j_4 j_2} \delta_{q m_1} \delta_{q m_2}}{\sqrt{(2J + 1)(2J' + 1)}} (-1)^{j_4 + j_2 + 2J} \langle \mu_4 || T_p || \lambda_4 \rangle \langle \mu || U_p || \lambda \rangle
\]

and obtain

\[
\langle (\mu_4 \lambda_4 || W^* || (\lambda_4 \mu) \rangle = \frac{\delta_{j_4 j_2} \delta_{q m_1} \delta_{q m_2}}{\sqrt{(2J + 1)(2r + 1)}} (-1)^{j_4 + j_2 + 2J} \langle \mu_4 || T_p || \lambda_4 \rangle \langle \mu || U_p || \lambda \rangle
\]

Angular momentum algebra, Wigner-Eckart theorem

The tensor operator in the nucleon-nucleon potential can be written as

\[
V = \frac{3}{2} \left[ r_0 \otimes r_0 \right] \otimes \left[ r \otimes r \right]
\]

Since the irreducible tensor \([ r \otimes r ] \) operates only on the angular quantum numbers and \([ r_0 \otimes r_0 ] \) operates only on the spin states we can write the matrix element

\[
\langle S \Sigma || V || S' \Sigma' \rangle = \langle S \Sigma || r_0 \otimes r_0 \rangle \langle r_0 \otimes r_0 || S' \Sigma' \rangle
\]

\[
= (-1)^{j_4 + j_2 + 2J} \langle \mu_4 || T_p || \lambda_4 \rangle \langle \mu || U_p || \lambda \rangle \times (S || r_0 || S')
\]

Angular momentum algebra, Wigner-Eckart theorem

We need that the coordinate vector \( r \) can be written in terms of spherical harmonics as

\[
r_n = r_n \frac{\sqrt{2n+1}}{\sqrt{Y_n}} Y_n
\]

Using this expression we get

\[
[r \otimes r]^{(2)} = \frac{4 \pi}{3} \sum_{n, l} \langle 2l+1 || 2n || 2l || Y_n || Y_n \rangle
\]

Angular momentum algebra, Wigner-Eckart theorem

The product of two spherical harmonics can be written as

\[
Y_{l_1 m_1} Y_{l_2 m_2} = \sum_{m} \sqrt{\frac{(2l_1+1)(2l_2+1)(2l+1)}{4\pi}} \left( \frac{h_l}{m_l} \frac{b_l}{m_l} \right) Y_{l m} (-1)^m
\]

\[
\times \left( \begin{array}{c} h_l \ b_l \\ 0 \ 0 \end{array} \right) \ Y_{l m} (-1)^m.
\]
Transformations from the relative and center-of-mass motion system to the lab system will be discussed below.

To obtain a $V$-matrix in a h.o. basis, we need the transformation

$$\langle nNLST' | V | n'NL'L'S'T \rangle,$$

with $n$ and $N$ the principal quantum numbers of the relative and center-of-mass motion, respectively.

$$\langle nNLST | V^2 | n'NL'L'S'T \rangle = \int k^2 dk K_{nl}(\sqrt{2\alpha k})K_{nl}(\sqrt{2\alpha k})|\langle nNLST | V | n'NL'L'S'T \rangle|^2.$$

The parameter $\alpha$ is the chosen oscillator length.

The most commonly employed $V$-basis is the harmonic oscillator, which in turn means that a two-particle wave function with total angular momentum $J$ and isospin $T$ can be expressed as

$$\langle nNLST | V | n'NL'L'S'T \rangle = \frac{1}{\sqrt{(1+\alpha)^{15}}} \sum_{F} \sum_{J} \sum_{S} \sum_{T} \left\{ F \right\} \left\{ J \right\} \left\{ S \right\} \left\{ T \right\} \times (-1)^{F-J-S-T} \langle \alpha || J || S || T \rangle \times \langle nNLST' | V | n'NL'L'S'T \rangle.$$

where the term $\langle nNLST | V | n'NL'L'S'T \rangle$ is the so-called Moshinsky-Talmi transformation coefficient (see chapter 18 of Alex Brown’s notes).
The term $\langle ab|LSJ \rangle$ is a shorthand for the $LS - jj$ transformation coefficient,
$$
\langle ab|LSJ \rangle = \hat{J}_S \hat{J}_J \hat{L} \hat{s}_a \hat{s}_b \hat{S} \hat{j}_a \hat{j}_b \lambda \, S \, J.
$$
Here we use $\hat{x} = \sqrt{2x + 1}$. The factor $F$ is defined as
$$
F = 1 - (-1)^{l + S + T} \sqrt{2} \text{ if } s_a = s_b \text{ and we}
$$