## group theory - week 12

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### Georgia Tech PHYS-7143

**Homework HW12** due Tuesday, April 12, 2016

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== show all your work for maximum credit,
== put labels, title, legends on any graphs
== acknowledge study group member, if collective effort
== if you are LaTeXing, here is the source code

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Exercise 12.1 *Splitting of degeneracies in a central potential* 5 points
Exercise 12.2 *Quadrupole transitions* 5 points

Total of 10 points = 100 % score.

### 2016-04-05 Boris Lecture 22 Clebsch-Gordon coefficients. Wigner-Eckart theorem

Gutkin notes, Lect. 9 *SU(2), SO(3) and their representations*, Sects. 5-8

### 2016-04-07 Boris Lecture 23 Immer Mehr Gruppenpest

Gutkin notes, Lect. 9 *SU(2), SO(3) and their representations*: Zeeman effect.

Gutkin notes, Lect. 10 *Representations of simple algebras, general construction. Application to SU(3)*, Sects. 1-4.

## 12.1 Some applications of group theory to quantum mechanics

K. Y. Short

As a typical example, consider the correspondence between $SU(2)$ and $SO(3)$ with applications to quantum mechanics.

Angular momentum $L = r \times p$ has three components, the operators that generate $SU(2)$ and satisfy $[L_1, L_2] = iL_3$. If we define $e = L_1 + iL_2$, $f = L_1 - iL_2$, and $h = 2L_3$, then we have the following algebra:

$$[h, e] = 2e, \quad [h, f] = -2f, \quad [e, f] = h \tag{12.1}$$

where

$$e = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad f = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \quad h = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{12.2}$$

Clearly $e$ and $f$ act as the raising and lowering (also called 'ladder') operators $L_\pm$ in this representation.

We observe that there are $n^2 - 1 = 3$ such operators satisfying this algebra, which is the Lie algebra of SU(n), where $n = 2$. The eigenvalues of $h$ are integers separated by 2, and the eigenvalues of $L_3$ must be half-integers separated by 1. Consequently, the representation with highest $L_3$ eigenvalue given by $l$ must have dimension $2l + 1$ (note: $2l$ is $\lambda_{max}$ for $h$).

Further, $L^2 = L \cdot L$ commutes with $L_1$, $L_2$, and $L_3$ and hence, by Schur's Lemma, $L^2 = \lambda \mathbb{I}$ in this representation, so every vector is an eigenvector of $L^2$. For example, we've seen in quantum mechanics,

$$L^2 \, Y_l^m = l(l+1)\hbar^2 \, Y_l^m \tag{12.3}$$

And since the spherical harmonics $Y_l^m(\theta, \phi)$ constitute an orthonormal basis of the Hilbert space of square-integrable functions, any vector can be expanded in a basis of $Y_l^m(\theta, \phi)$. $L_\pm$ act on $Y_l^m$ in the following way:

$$L_\pm Y_l^m = \hbar\sqrt{l(l+1) - m(m \pm 1)} \, Y_l^{m\pm 1} \tag{12.4}$$

And so we see that the $2 \times 2$ matrices of $SU(2)$ have a relation to the spherical harmonics.

An element of $SU(2)$ can be written as

$$e^{i\sigma_j\alpha_j/2} \tag{12.5}$$

where $\sigma_j$ is a Pauli matrix and $\alpha_j$ is a number. (The exponentiation of the Pauli matrices gives $SU(2)$.) We will now work to understand the importance of the$1/2$ factor in the argument of the exponential. First, consider a generic position vector $\boldsymbol{r} = x\hat{e}_i + y\hat{e}_j + z\hat{e}_k$. We may construct a matrix of the form

$$\begin{aligned}\sigma \cdot r &= \sigma_x x + \sigma_y y + \sigma_z z \\ &= \begin{pmatrix} 0 & x \\ x & 0 \end{pmatrix} + \begin{pmatrix} 0 & -iy \\ iy & 0 \end{pmatrix} + \begin{pmatrix} z & 0 \\ 0 & -z \end{pmatrix} \\ &= \begin{pmatrix} z & x-iy \\ x+iy & -z \end{pmatrix}\end{aligned} \tag{12.6}$$

Taking the determinant,

$$\det \begin{pmatrix} z & x-iy \\ x+iy & -z \end{pmatrix} = -(x^2+y^2+z^2) = -\boldsymbol{x}^2 \tag{12.7}$$

which gives an expression for the length of a vector.

Now consider a unitary transformation of this matrix. For example,

$$\begin{aligned}U(\sigma \cdot r)U^\dagger &= \sigma_x(\sigma \cdot r)\sigma_x \\ &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} z & x-iy \\ x-iy & z \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\ &= \begin{pmatrix} -z & x+iy \\ x-iy & z \end{pmatrix}\end{aligned} \tag{12.8}$$

Taking this determinant, we find the same expression as before:

$$\det \begin{pmatrix} -z & x+iy \\ x-iy & z \end{pmatrix} = -(x^2+y^2+z^2) = -\boldsymbol{x}^2 \tag{12.9}$$

We observe that, like $SO(3)$, $SU(2)$ preserves the lengths of vectors.

The correspondence between $SO(3)$ and $SU(2)$ can be made more explicit. To see this, consider an $SU(2)$ transformation on a two-component object called a *spinor* $\psi$ where

$$\psi = \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \tag{12.10}$$

With

$$x = \frac{1}{2}(\beta^2 - \alpha^2), \quad y = -\frac{i}{2}(\alpha^2 + \beta^2), \quad z = \alpha\beta \tag{12.11}$$

One may check that an $SU(2)$ transformation on $\psi$ is equivalent to an $SO(3)$ transformation on $\boldsymbol{x}$. From this equivalence, one sees that an $SU(2)$ transformation has three real parameters that correspond to the three rotation angles of $SO(3)$. If we label the "angles" for the $SU(2)$ transformation by $\alpha$, $\beta$, and $\gamma$, we observe, for a "rotation" about $\hat{x}$

$$U_x(\alpha) = \begin{pmatrix} \cos\alpha/2 & i\sin\alpha/2 \\ i\sin\alpha/2 & \cos\alpha/2 \end{pmatrix} \tag{12.12}$$

Likewise for an $SU(2)$ transformation about $\hat{y}$:

$$U_y(\beta) = \begin{pmatrix} \cos\beta/2 & \sin\beta/2 \\ -\sin\beta/2 & \cos\beta/2 \end{pmatrix} \tag{12.13}$$

And for the final rotation, the $SU(2)$ transformation about $\hat{z}$:

$$U_z(\gamma) = \begin{pmatrix} e^{i\gamma/2} & 0 \\ 0 & e^{-i\gamma/2} \end{pmatrix} \tag{12.14}$$

Compare these three matrices to the corresponding $SO(3)$ rotation matrices:

$$R_x(\zeta) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\zeta & \sin\zeta \\ 0 & -\sin\zeta & \cos\zeta \end{pmatrix}, \quad R_y(\phi) = \begin{pmatrix} \cos\phi & 0 & \sin\phi \\ 0 & 1 & 0 \\ -\sin\phi & 0 & \cos\phi \end{pmatrix}$$
$$R_z(\theta) = \begin{pmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{12.15}$$

They're equivalent! Result: **Half the rotation angle generated by $SU(2)$ corresponds to a rotation generated by $SO(3)$.**

Neat fact: Gauge bosons corresponding to the $SU(2)$ symmetry are the $W$ and $Z$ bosons that carry the weak interaction.

In this context, the eigenvalue equation for $L_3$ and for $L^2$ are differential equations whose solutions are the spherical harmonics $Y_l^m$ which take the form

$$e^{im\phi}P_l^m(\cos\theta), \quad -l \leq m \leq l \tag{12.16}$$

in spherical coordinates and which determine the shape of electron orbitals and their probabilities to be found in a given region.

In quantum mechanics, the possible results of a measurement are determined by the possible eigenvalues of an operator. As such, the possible measurable values of the $z$-component of angular momentum correspond to the allowed values of $L_3$. The measurement outcomes are not arbitrary; the largest one, $l$, must be a half-integer, and there are $2l+1$ eigenvectors. Applying the lowering operator $L_-$ one-by-one, we can find the possible outcomes to be $m \in \{l, l-1, ..., -l\}$. The angular dependence of the corresponding wave function goes as $\sim e^{im\phi}P_l^m(\cos\theta)$. In addition, higher values of $l$ correspond to higher energy, so the different values of $l$ correspond to different electron orbitals in order of increasing energy.

note: The set $\{e, f, h\}$ forms an '$sl_2$-triple'.

# Exercises

12.1. **Splitting of degeneracies in a central potential.** Hamiltonian $H_0$ has rotational symmetry of $SO(3)$.

(a) What are the possible energy level degeneracies of $H_0$?

A weak perturbation $V$ with a symmetry $T_d$ of full tetrahedron group is added (e.g., $V$ is a potential created by lattice of atoms with a symmetry of $T_d$).

(b) What will be the degeneracies of new Hamiltonian $H_0 + V$?

(c) Assuming that the total angular momentum of the system before the perturbation is $l = 2$. How the degeneracies of the corresponding energy level will be split after the perturbation is applied?

(B. Gutkin)

12.2. **Quadrupole transitions.**
a) Write $Q_1 = xy$, $Q_2 = zy$, $Q_3 = x^2 - y^2$ and $Q_4 = 2z^2 - x^2 - y^2$ as components of spherical tensor of rank 2. *Hint:* use spherical harmonics $Y_l^m(\theta, \varphi)$.
b) The last quantity $Q_4$ is known as quadrupole moment. What are the selection rules for transitions induced by $Q_4$ in a system with $SO(3)$ symmetry? In other words, for which $m, l$ and $k, j$ the transition rates:

$$P_{m,l \to k,j} \sim |\langle m\, l|Q_4|j\, k\rangle|^2$$

are non-zero?
c) By using Wigner-Eckart theorem write down the relationship between $|\langle m\, l|Q_4|j\, k\rangle|^2$ and $|\langle m\, l|Q_1|j\, k\rangle|^2$ in terms of Clebsch-Gordan coefficients.

(B. Gutkin)