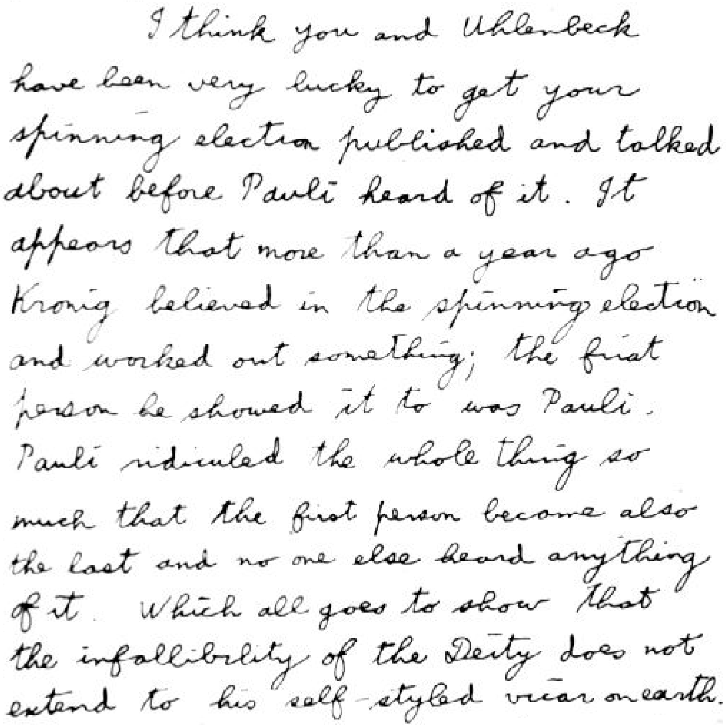
Module II, Lecture 04: *SU*(*N*) Unitary Groups

Historical notes

A number of experimental observations reported in 1920-es have led to a conjecture that the electron has an intrinsic magnetic moment that is distinct from the one associated with its orbital motion. The intrinsic magnetic moment hypothesis yielded a satisfactory explanation of the anomalous Zeeman effect, of the fine structure of atomic spectra of alkali metals and of some other observations. In 1925, Uhlenbeck and Goudsmit proposed an explanation for this magnetic moment, suggesting that the electron has an intrinsic angular momentum, which they called *spin*.


I think you and Uhlenbeck have been very lucky to get your spinning electron published and talked about before Pauli heard of it. It appears that more than a year ago Kronig believed in the spinning electron and worked out something; the first person he showed it to was Pauli. Pauli ridiculed the whole thing so much that the first person became also the last and no one else heard anything of it. Which all goes to show that the infallibility of the Deity does not extend to his self-styled vicar on earth.

Part of a letter by L.H. Thomas to Samuel Goudsmit (25 March 1926).

This proposal faced serious difficulties. It contradicted the notion of elementary particle as a "point" object – as previously understood, a point particle could not "rotate". The spin hypothesis did not fit into Schrödinger's wavefunction formalism either – the experiment by Stern and Gerlach suggested that an electron in a magnetic field can only have two "spin states", which meant that the corresponding operator must have *exactly two* eigenfunctions. Because angular momentum was assumed to be involved, the spin operators had to come from some representation of $SO(3)$. However irreducible representations of $SO(3)$ have dimensions of $2j+1$. So j had to be set to a fractional value, meaning that the resulting space had a bizarre physical interpretation (a wavefunction that changes sign upon a 360-degree rotation). For this reason, the angular momentum analogy for spin is deeply misleading – a much neater construction is presented below from purely algebraic considerations.

Introducing *SU*(*N*)

Ironically (see the letter above), the first description of spin was constructed by Pauli, who suggested that a discrete spin variable be introduced into the wavefunction as a separate coordinate

$$\psi(x,y,z) \quad \to \quad \psi(x,y,z,\sigma), \qquad \sigma = 1,2,3...$$

and the infinite-dimensional Hilbert space of wavefunctions be crossed with a $(2j+1)$-dimensional spin space (elements of this space became known as *spinors*):

$$\mathbb{C}^{\infty} \quad \to \quad \mathbb{C}^{\infty} \otimes \mathbb{C}^{2j+1}$$

with some norm-preserving (*i.e.* unitary) time propagators defined on $\mathbb{C}^{2j+1}$.

The Lie group of all unitary operators driving time dynamics on $\mathbb{C}^{2j+1}$ is $SU(2j+1)$ and the corresponding Lie algebra of Hermitian operators is $\mathfrak{su}(2j+1)$. In the simplest case of spin-1/2, we get

$SU(2)$, which fits our bill simply because it is the most general group describing the dynamics of a two-level quantum system. This simple explanation is in sharp contrast with the prevailing confusion (particularly amongst the so-called "philosophers of physics") regarding the role of $SU(2)$, which is exacerbated by the fact that $\mathfrak{so}(3)$ and $\mathfrak{su}(2)$ Lie algebras are isomorphous – their basis operators obey the same commutation relations, meaning that the structure coefficients happen to be the same.

Similarly, the Lie group describing the dynamics of a particle with three distinct energy levels is in general $SU(3)$. Many particle physics textbooks insist that particles of different total spin are described by different irreducible representations of $SU(2)$ – this is true for an isolated spin in vacuum because some transitions are degenerate and cannot be accessed independently, but this is not the case in Magnetic Resonance, where energy levels are shifted and mixed by various interactions, and so in practice the dynamical group of a spin-j particle in Magnetic Resonance is $SU(2j+1)$. For spin-1 particle it is easy to show that the Zeeman and quadrupolar interaction operators:

$$\left\{\hat{L}_{\mathrm{X}},\ \hat{L}_{\mathrm{Y}},\ \hat{L}_{\mathrm{Z}},\ \hat{L}_{\mathrm{X}}^2,\ \hat{L}_{\mathrm{Y}}^2,\ \hat{L}_{\mathrm{X}}\hat{L}_{\mathrm{Z}},\ \hat{L}_{\mathrm{Y}}\hat{L}_{\mathrm{Z}},\ \hat{L}_{\mathrm{Z}}^2-\frac{2}{3}\hat{E}\right\}$$

are actually linear combinations of the eight Gell-Mann matrices, and the algebra that is spanned by the resulting basis is $\mathfrak{su}(3)$. In the context of Magnetic Resonance spectroscopy, the role of $SU(2)$ in defining the state space dimension for particles of different spin is accidental – $SU(2)$ simply happens to have irreducible representations of every dimension.

Cartan subalgebras, roots and weights

If $\mathfrak{g}$ is a semisimple Lie algebra and $\mathfrak{h}\subset\mathfrak{g}$ is its largest Abelian subalgebra, then $\mathfrak{h}$ is called a *Cartan subalgebra* of $\mathfrak{g}$. Because all elements of $\mathfrak{h}$ commute, they may be simultaneously diagonalized. In the resulting set of diagonal matrices $H\in span\{H_1,\ldots,H_k\}$, where $\{H_1,\ldots,H_k\}$ is some basis set, the eigenvalues at a specific position j along the diagonal are called *weights* and denoted $\mu_j(H)$. A weight is a linear functional on $\mathfrak{h}$:

$$\mu_j(\alpha A+\beta B)=\alpha\mu_j(A)+\beta\mu_j(B),\qquad A,B\in\mathfrak{h},\qquad \alpha,\beta\in\mathbb{C}$$

Vectors of the form $\vec{\mu}_j=\begin{bmatrix}\mu_j(H_1) & \ldots & \mu_j(H_k)\end{bmatrix}$ are called *weight vectors* and the space they span a *weight space*. Lie algebra weights occurring in its adjoint representation are called *roots* and the corresponding space a *root space*.

Roots and weights of $\mathfrak{su}$(2) and $\mathfrak{su}$(3)

As an illustration to the definitions above we will consider the simplest cases of $\mathfrak{su}(2)$ and $\mathfrak{su}(3)$ Lie algebras. $\mathfrak{su}(2)$ is a fairly easy case, specifically:

1. There is only one diagonal generator ($\hat{L}_{\mathrm{Z}}$) and its eigenvalues are weights – they are scalars and correspond to the physically allowed projections of spin on the Z axis:

   $$\hat{L}_{\mathrm{Z}}\left|S,\mu\right\rangle=\mu\left|S,\mu\right\rangle$$

   where S enumerates the irreducible representations and μ is the weight.

2. Irreducible representations of $SU(2)$ can be labelled by the highest weight, *i.e.* by the maximum projection quantum number allowed: $S=$1/2, 1, 3/2, 2, *etc.*

3. Only one type of operator ($\hat{L}_+$ and its conjugate) is needed to move between weights.

In $\mathfrak{su}(3)$ there are eight generators (the Gell-Mann matrices listed below are a good practical choice because they generalize Pauli matrices) of which two are diagonal:

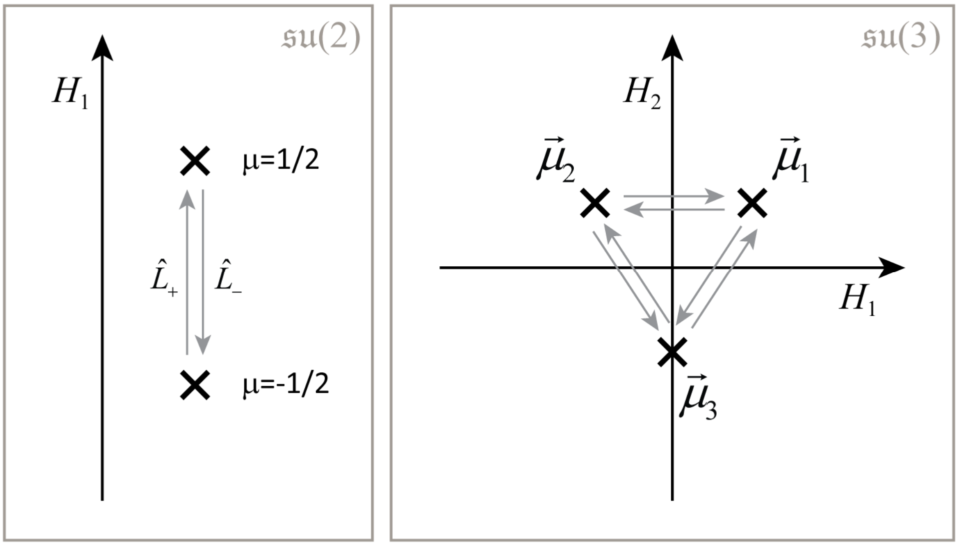
$$\lambda_1 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \qquad \lambda_2 = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \qquad \lambda_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \qquad \lambda_4 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}$$

$$\lambda_5 = \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix} \qquad \lambda_6 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \qquad \lambda_7 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix} \qquad \lambda_8 = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}$$

and so the weights are 2-vectors:

$$\hat{H}_1 \left| D, \vec{\mu} \right\rangle = \mu_1 \left| D, \vec{\mu} \right\rangle \qquad \hat{H}_2 \left| D, \vec{\mu} \right\rangle = \mu_2 \left| D, \vec{\mu} \right\rangle \qquad \hat{H}_1 = \lambda_3 \quad \hat{H}_2 = \lambda_8$$

where D enumerates the irreducible representation. Instead of the nice vertical diagram that we had for $\mathfrak{su}(2)$, we now have weights arranged on a 2D plane:



where the weight vectors are listing the eigenvalues of the three state vectors with respect to the two basis operators of the Cartan subalgebra:

$$\vec{\mu}_1 = \begin{pmatrix} \frac{1}{2} & \frac{\sqrt{3}}{6} \end{pmatrix} \qquad \vec{\mu}_2 = \begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{6} \end{pmatrix} \qquad \vec{\mu}_3 = \begin{pmatrix} 0 & -\frac{\sqrt{3}}{3} \end{pmatrix}$$

and transitions between them are accomplished using the $\mathfrak{su}(3)$ equivalents of raising and lowering operators. They are no longer just raising and lowering, but they serve the same purpose. The diagrams above refer to the fundamental representations of $\mathfrak{su}(2)$ and $\mathfrak{su}(3)$ – representations of greater dimension would have more complex diagrams with a greater number of weights.

The weights in the adjoint representation are called roots. For the familiar case of $\mathfrak{su}(2)$ the adjoint representation is three-dimensional and the eigenoperators of the $\hat{L}_Z$ commutation superoperator are:

$$[\hat{L}_Z,\hat{L}_Z]=0 \qquad [\hat{L}_Z,\hat{L}_+]=\hat{L}_+ \qquad [\hat{L}_Z,\hat{L}_-]=-\hat{L}_-$$

and so the roots of $\mathfrak{su}(2)$ are 0, 1 and –1.

Multi-spin systems

Because the state space of a multi-spin system is a direct product of state spaces of individual spins, the algebra of operators acting on the state space of a multi-spin system is a direct product of single-spin operator algebras. In the case of a two-spin system with both spins ½, the direct product algebra $\mathfrak{su}(2)\otimes\mathfrak{su}(2)$ has 15 basis operators (identity is not an element of a Lie algebra):

	$\hat{E}$	$\hat{S}_X$	$\hat{S}_Y$	$\hat{S}_Z$
$\hat{E}$	$\hat{E}\otimes\hat{E}$	$\hat{E}\otimes\hat{S}_X$	$\hat{E}\otimes\hat{S}_Y$	$\hat{E}\otimes\hat{S}_Z$
$\hat{L}_X$	$\hat{L}_X\otimes\hat{E}$	$\hat{L}_X\otimes\hat{S}_X$	$\hat{L}_X\otimes\hat{S}_Y$	$\hat{L}_X\otimes\hat{S}_Z$
$\hat{L}_Y$	$\hat{L}_Y\otimes\hat{E}$	$\hat{L}_Y\otimes\hat{S}_X$	$\hat{L}_Y\otimes\hat{S}_Y$	$\hat{L}_Y\otimes\hat{S}_Z$
$\hat{L}_Z$	$\hat{L}_Z\otimes\hat{E}$	$\hat{L}_Z\otimes\hat{S}_X$	$\hat{L}_Z\otimes\hat{S}_Y$	$\hat{L}_Z\otimes\hat{S}_Z$

and generates $SU(2)\otimes SU(2)$ Lie group under the exponential map. Similarly, the dynamics of a pair of spin-1 particles would in general be governed by $SU(3)\otimes SU(3)$, *etc*. In practical calculations of multi-spin systems (particularly in Product Operator Formalism) $\hat{A}\otimes\hat{B}$ is often abbreviated $\hat{A}\hat{B}$, but only if the symbols used for the operators for the two spins are different.

Relationship between *SU*(2) and *SO*(3)

In the context of magnetic resonance, $SO(3)$ is the group of *rotations in real physical space* – it refers to the rotation of molecules and various interaction parameters, such as inter-nuclear vectors. These rotation operators *do not affect spin* – as we noted in the previous lecture, the spin projections on the laboratory frame axes are not changed during molecular rotations. Therefore, $SO(3)$ governs rotations and angular momentum, but not spin.

In contrast to the above, $SU(2)$ is the group of *unitary transformations of spin wavefunction space*, having nothing to do with rotations of the real physical space. $SU(2)$ operators create and modify linear combinations of spin wavefunctions, which may sometimes be visualized as rotations between some basis functions, but more often cannot be. For a unitary transformation of wavefunctions in a given basis, the proposition that $\psi(\varphi)=-\psi(\varphi+2\pi)$ with respect to some mixing angle φ is no longer ridiculous, and half-integer eigenvalues for $\hat{L}^2$ and $\hat{L}_Z$ may actually be allowed if that is what the experimental results demand.

Because their algebras are isomorphous, the mapping between $SU(2)$ and $SO(3)$ is locally an isomorphism, but globally the exact relationship is that the factor group $SU(2)/C_2$ is isomorphous to $SO(3)$, where C_2 is the permutation group of two objects. This is known as “double cover” and means that two different elements of $SU(2)$ correspond to each element of $SO(3)$.

Universal enveloping algebra of $\mathfrak{su}(2)$

In practical spin dynamics simulations one often finds that having just $\{\hat{L}_{\mathrm{X}}, \hat{L}_{\mathrm{Y}}, \hat{L}_{\mathrm{Z}}\}$ as the basis set and just the Lie bracket as an operation is not sufficient – extra operators are required for physical reasons, such as the non-Hermitian raising and lowering operators $\hat{L}_{\pm} = \hat{L}_{\mathrm{X}} \pm i\hat{L}_{\mathrm{Y}}$, as well as powers (rather than commutators) of the basis operators, which do not belong to $\mathfrak{su}(2)$. The operator describing nuclear quadrupolar interaction, for example

$$\hat{H}_{\mathrm{Q}} = \frac{3e^2 qQ}{4L(2L-1)\hbar}\left\{\left(\hat{L}_{\mathrm{Z}}^2 - \frac{1}{3}\hat{L}^2\right) + \frac{\eta}{3}\left(\hat{L}_{\mathrm{X}}^2 - \hat{L}_{\mathrm{Y}}^2\right)\right\}$$

contains powers of the basis operators. This is an often encountered situation, which may be formally accommodated (whilst preserving the representation structure) by allowing the simple associative product in the original Lie algebra. The resulting associative algebra is called *universal enveloping algebra* (or simply *envelope*) of the original Lie algebra. The raising and lowering operators $\hat{L}_{\pm}$, their various powers as well as the total spin operator $\hat{L}^2$ live in the envelope of $\mathfrak{su}(2)$.