

# Quantum Information Theory Introduction

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# Abstract

I will generalize the Pauli Matrices to the Gell Mann Matrices. I will discuss some identities of the Gell Mann Matrices. I will discuss Lie Algebras. I will discuss the generators of a Lie Algebra. I will discuss Ritter's decomposition of a density matrix into a polynomial in symmetrized products of Lie algebra generators. I will discuss the FMO complex and the relationship of the FMO complex to QIT.

## Recall

From a previous lecture we recall that...

- ▶ ...a semigroup of quantum channels maps positive semidefinite trace 1 density matrices to other density matrices by conjugation by Kraus operators or an affine transformation of a Bloch vector of Pauli matrix weights.

$$\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

- ▶ ...the Von Neumann entropy is defined as  $-Tr(\rho \log_2(\rho))$ .
- ▶ ...the Holevo capacity was shown to be non-additive by M.B. Hastings.

$$\chi(\Phi_1 \otimes \Phi_2) \neq \chi(\Phi_1) + \chi(\Phi_2)$$

# Gell Mann Matrices

Spin 1 systems are described by a set of 3x3 matrices called the Gell Mann matrices which generalize the Pauli matrices.

$$\begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}$$
$$\begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix} \quad \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$$
$$\begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix} \quad \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix} \quad \begin{pmatrix} \frac{1}{\sqrt{3}} & 0 & 0 \\ 0 & \frac{1}{\sqrt{3}} & 0 \\ 0 & 0 & \frac{-2}{\sqrt{3}} \end{pmatrix}$$

They are traceless Hermitian matrices. The three pairs of off diagonal matrices each generate linear combinations of the diagonals.

# Gell Mann Matrix Expansion of Density Matrices

Any Hermitian matrix can be written as a real linear combination of the generalized  $n$ -dimensional Gell Mann matrices along with the identity.

$$\rho = \frac{1}{3}(I + w_1 \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} + w_2 \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} + w_3 \begin{pmatrix} 0 & -z & 0 \\ z & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} + w_4 \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \\ + w_5 \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} + w_6 \begin{pmatrix} 0 & 0 & -z \\ 0 & 0 & 0 \\ z & 0 & 0 \end{pmatrix} + w_7 \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -z \\ 0 & z & 0 \end{pmatrix} + w_8 \begin{pmatrix} \frac{1}{\sqrt{3}} & 0 & 0 \\ 0 & \frac{1}{\sqrt{3}} & 0 \\ 0 & 0 & \frac{-2}{\sqrt{3}} \end{pmatrix})$$

The eigenvalues can be written in terms of the weights of these matrices, but not in a human readable way. The description of the Bloch manifold of density matrices is not necessarily spherical for  $n > 2$ .

## Commutators of Gell Mann Matrices and Structure Constants

The commutator  $[x, y]$  of any two Gell Mann Matrices  $x, y$  can be written  $xy - yx = kg$  for some Gell Mann Matrix  $g$  and complex  $k$ .

$$\begin{aligned} & \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 0 & -z & 0 \\ z & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} - \begin{pmatrix} 0 & -z & 0 \\ z & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \\ &= z \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix} - -z \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix} = 2z \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \end{aligned}$$

The constant  $k/i$  is called a structure constant and can be computed readily for all pairs.

$$\begin{aligned} & \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} - \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \\ &= \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix} - \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} = z \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -z \\ 0 & z & 0 \end{pmatrix} \end{aligned}$$

The structure constants for the Gell Mann Matrices form a completely antisymmetric tensor and have values including 0, 1,  $\frac{1}{2}$ , and  $\frac{\sqrt{3}}{2}$ . The structure constants are invariant under similarity transformations of the set of matrices.

# Generalized Gell Mann Matrices

Spin 3/2 systems are described by a set of 4x4 matrices...

$$\begin{pmatrix} 0 & -z & 0 & 0 \\ z & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}
 \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}
 \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}
 \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}$$

$$\begin{pmatrix} 0 & 0 & -z & 0 \\ 0 & 0 & 0 & 0 \\ z & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}
 \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & -z & 0 \\ 0 & z & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}
 \begin{pmatrix} \frac{1}{\sqrt{3}} & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{3}} & 0 & 0 \\ 0 & 0 & \frac{-2}{\sqrt{3}} & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}
 \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

$$\begin{pmatrix} 0 & 0 & 0 & -z \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ z & 0 & 0 & 0 \end{pmatrix}
 \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -z \\ 0 & 0 & 0 & 0 \\ 0 & z & 0 & 0 \end{pmatrix}
 \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -z \\ 0 & 0 & z & 0 \end{pmatrix}
 \begin{pmatrix} \frac{1}{\sqrt{6}} & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{6}} & 0 & 0 \\ 0 & 0 & \frac{1}{\sqrt{6}} & 0 \\ 0 & 0 & 0 & \frac{-3}{\sqrt{6}} \end{pmatrix}$$

Previous Gell-Mann matrices are recycled into the next generation.

In general, the rightmost diagonal matrix is given by

$$\sqrt{\frac{2}{d(d-1)}}(I_{d-1} \oplus (1-d))$$

# Commutators of Generalized Gell Mann Matrices and Structure Constants

In dimensions greater than three, the commutator  $[x, y]$  of any two generalized Gell Mann Matrices  $x, y$  can be written as a linear combination of Generalized Gell Mann Matrices with the coefficients generalizing the structure constants.

$$\begin{aligned} & \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -z \\ 0 & 0 & z & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} - \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -z \\ 0 & 0 & z & 0 \end{pmatrix} \\ & \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -z & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} - \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -z \end{pmatrix} \\ & \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -z & 0 \\ 0 & 0 & 0 & z \end{pmatrix} \end{aligned}$$

# Special Unitary Group

The Special Unitary Group of dimension  $n$  consists of determinant 1 unitary matrices acting on  $\mathbf{C}^n$ . The length of a vector  $s$  is invariant under transformations by the Special Unitary group. If  $U$  is a unitary matrix then the transformed state

$$\tilde{s} = Us$$

has length 1 if the original state has length 1.

$$s^* U^* Us = s^* s = 1$$

The set of unitary matrices for a given dimension is closed under composition, includes the identity matrix and contains the inverse of each of its members.  $SU(n)$  occurs frequently in the mathematical formulation of modern physics.

# Time Evolution of States and Matrices

In a closed system, if a state is evolved through time it reaches another state so time evolution preserves length. These operators can then be thought of as unitary operators. If  $\rho = ss^*$  is a density matrix representing some state  $s$  and  $U$  is a time evolution operator then

$$U\rho U^* = Uss^*U^*$$

is the same unitary matrix evolved through time. One must check linearity, invariance of the trace and total positivity, but time evolution can be thought of as a channel with  $\{U\}$  a Kraus operator.

# SU Channels

The set of special unitary channels or SU Channels are channels given by conjugation by special unitary matrices.

$$\{\Phi : \mathbf{B}(\mathbf{C}^n) \rightarrow \mathbf{B}(\mathbf{C}^m) \mid \Phi(\rho) = U\rho U^*, UU^* = I\}$$

These channels form a group that is studied for its relevance to physics.

# Lie Groups

A Lie Group  $G$  is a differentiable manifold with a group structure such that the group operation is continuous as a function from  $G \times G \rightarrow G$  and inversion is continuous.

- ▶ The Special Unitary group  $SU(n)$  is a Lie Group.

For every element  $g \in G$  of a Lie group there is an inner automorphism  $\Psi_g : G \rightarrow G$  given by conjugation by that element, denoted by  $\Psi_g(h) = ghg^{-1}$ .

# Lie Algebras

A Lie Algebra  $\mathfrak{g}$  is an associative algebra with a bilinear alternating bracket  $\{\}$  which satisfies the Jacobi identity. Every Lie Group  $G$  has an associated Lie Algebra  $\mathfrak{g}$ . The Lie Algebra  $\mathfrak{g}$  consists of those matrices  $g$  such that  $\exp g \in G$ .

- ▶ The Lie Algebra  $\mathfrak{su}(n)$  consists of those matrices  $h$  such that  $\exp h \in SU(n)$ . The algebra  $\mathfrak{su}(n)$  consists of traceless skew hermitian matrices with commutator as bracket.

## Theorem

*If  $h$  is traceless and skew hermitian  $\exp h$  will be special unitary.*

(First I show 'special') The eigenvalues of an exponential of a matrix will be the exponentials of the eigenvalues of the matrix. If the original matrix has trace zero  $\lambda_1 + \dots + \lambda_n = 0$ , then the exponential matrix will have determinant

$$\exp \lambda_1 \dots \exp \lambda_n = \exp (\lambda_1 + \dots + \lambda_n) = \exp 0 = 1$$

(Next 'Unitary') Since complex conjugation threads over sums and products,  $\exp (h)^* = \exp (h^*)$ . Then

$$\exp (h) \exp (h)^* = \exp (h) \exp (h^*) = \exp (h + h^*) = I$$

# Lie Algebra Generators and Tangent Space at the Identity

The exponential map can be written as the limit of a sequence of partial sums but also as a limit of a sequence of products.

$$\exp(h) = \lim_{n \rightarrow \infty} (I + h + h^2/2 + h^3/3! + \dots + h^n/n!)$$

$$\exp(h) = \lim_{n \rightarrow \infty} (I + h/n)^n$$

In this way, the elements of the Lie Algebra serve as infinitesimal generators of the Lie Group. Any Lie Algebra has a basis of infinitesimal generators of the Lie Group.

- ▶ The set of generalized  $n$  dimensional Gell Mann matrices in  $\mathfrak{su}(n)$  is a basis of the Infinitesimal Generators up to a multiple of  $i$ .

For this reason Lie Algebras are associated with the tangent space of the Lie Group at the identity  $T_I G$ .

## The Derivative of Conjugation

There is a map  $\Psi : G \rightarrow \text{Aut}(G)$  such that  $g \mapsto \Psi_g$ . The differential of this map at the identity element of the group in the direction of  $x$  can be calculated, yielding a map  $(d\Psi)_I : T_I(G) \rightarrow T_{\Psi(I)}(\text{Aut}(G))$ . The derivative of  $\Psi$  at the identity in the direction  $x$  applied to  $y$  is given by

$$\begin{aligned} & \lim_{\epsilon \rightarrow 0} \frac{\Psi(I+\epsilon x)[y] - \Psi(I)[y]}{\epsilon} \\ & \lim_{\epsilon \rightarrow 0} \frac{\Psi_{I+\epsilon x}[y] - \Psi_I[y]}{\epsilon} \\ & \lim_{\epsilon \rightarrow 0} \frac{(I+\epsilon x)y(I+\epsilon x)^{-1} - y}{\epsilon} \\ & \lim_{\epsilon \rightarrow 0} \frac{(I+\epsilon x)y(I-\epsilon x + (\epsilon x)^2 + O(\epsilon^3)) - y}{\epsilon} \\ & \lim_{\epsilon \rightarrow 0} \frac{((I+\epsilon x)y - (I+\epsilon x)y\epsilon x + (I+\epsilon x)y(\epsilon x)^2 + O(\epsilon^3)) - y}{\epsilon} \\ & \lim_{\epsilon \rightarrow 0} \frac{((Iy + \epsilon xy) - (Iy\epsilon x + \epsilon xy\epsilon x) + (Iy(\epsilon x)^2 + \epsilon xy(\epsilon x)^2) + O(\epsilon^3)) - y}{\epsilon} \\ & \lim_{\epsilon \rightarrow 0} \frac{(y + \epsilon xy - y\epsilon x - \epsilon xy\epsilon x + y(\epsilon x)^2 + \epsilon xy(\epsilon x)^2 + O(\epsilon^3)) - y}{\epsilon} \\ & \lim_{\epsilon \rightarrow 0} (xy - yx - \epsilon xyx + y(\epsilon)(x)^2 + \epsilon xy(\epsilon x) + O(\epsilon^2)) \end{aligned}$$

$$(xy - yx) = [x, y]$$

The derivative operator  $d(\Psi_I)_x : T_x(G) \rightarrow T_{\Psi_I(x)}(G)$  can be thought of as a map from  $\mathfrak{g} \rightarrow \mathfrak{g}$  because  $T_{\Psi_I(x)}(G) = T_x(G) = \mathfrak{g}$ . So the derivative of the conjugation operator in the Lie Group is the Lie Bracket of the Lie Algebra.

# Ritter's Decomposition

Given the set of generalized Gell Mann Matrices, any density matrix may be written as

$$\rho = \sum_i (w_i GM_i) / n$$

for some weights  $w_i$  where  $w_0$  corresponding to the identity matrix equals 1.

Theorem 6 of Ritter [2] shows that states may also be written

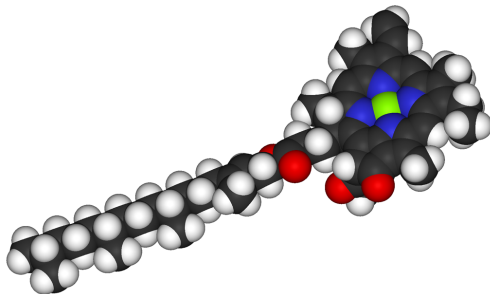
$$\rho = \sum_i w_i X_i + \sum_{i,j} w_{i,j} X_i X_j + \sum_{i,j,k} w_{i,j,k} X_i X_j X_k + \dots$$

where  $X_i$  is an infinitesimal generator and the set of  $X_i$ s are a fundamental representation of the Lie Algebra.

$$x_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \quad x_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & -z & 0 \\ z & 0 & -z \\ 0 & z & 0 \end{pmatrix} \quad x_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

# Chlorophyll

Chlorophyll is a molecule used by plants and bacteria create useful

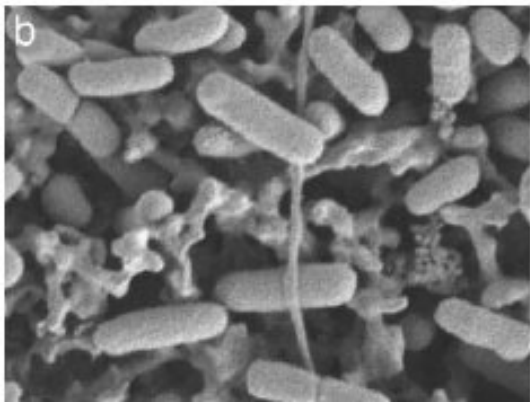


chemical energy.

There are many forms of Chlorophyll. When a photon hits a Chlorophyll molecule, the molecule becomes excited. This excitement can be passed to other molecules. This excited molecule is called an exciton.

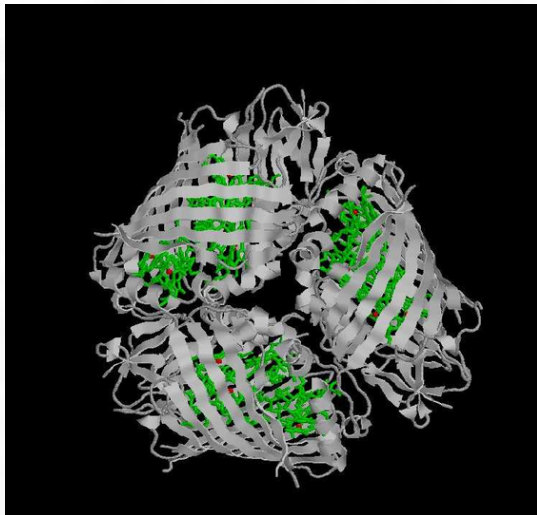
## Green Sulfur Bacteria

*Chlorobium Tepidum*, or Green Sulfur Bacteria, possess a particular kind of chlorophyll arranged in complexes named after Fenna-Matthews-Olson. These complexes are localized in packets of hundreds of thousands of chlorophyll molecules called chlorosomes. These harvest light so efficiently that bacteria can live in the dim glow of an underwater volcano or hundreds of feet below the water's surface.



## Fenna-Matthews-Olson

In Green Sulfur Bacteria, the FMO is a trimer made of identical subunits containing seven bacteriochlorophyll a (BChl-a) molecules. They transfer excitons from the chlorosomes to the membrane reaction center in Excitation Energy Transfer (EET).



## Fenna-Matthews-Olson Model

In creating our quantum model, we first might consider  $2^7$ -dimensional vectorspaces, with one choice for each state of the molecule. This is intractable so we make a simplifying assumption; over small time scales any of the chlorophyll molecules could be excited, but only one of the seven molecules will be excited at any one time. The excitation evolution has been modeled as a markov chain and a coherent quantum state in a seven dimensional vector space.





$$\begin{pmatrix} ? & ? & ? & ? & ? & ? & ? \\ ? & ? & ? & ? & ? & ? & ? \\ ? & ? & ? & ? & ? & ? & ? \\ ? & ? & ? & ? & ? & ? & ? \\ ? & ? & ? & ? & ? & ? & ? \\ ? & ? & ? & ? & ? & ? & ? \\ ? & ? & ? & ? & ? & ? & ? \end{pmatrix}$$

How can we use Quantum Information Theory to gain information about this physical system?


## Summary

Generalized the Pauli Matrices to the Gell Mann Matrices. The Commutator of any two Gell Mann Matrices is a linear combination of Gell Mann Matrices. For every Lie Group, one can associate the Lie Algebra with the tangent space to the Group at the identity. A Lie Algebra can be generated by a smaller set. Ritter's decomposition of a density matrix into a polynomial in symmetrized products of Lie algebra generators allowed him to explicitly compute certain channels in higher dimensions. QIT provides a framework for working with physical systems like the FMO complex of Green Sulfur Bacteria.

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