D'Seminar course

Non-commutative analysis and symmetry

Lecture + extra

Introduction to Lie algebras and Lie groups

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A Lie algebra over field $K$ is called a Lie algebra over field $K$ if:

1. $L$ is a linear space over $K$.
2. $\langle \cdot, \cdot \rangle : L \times L \to L$ is a bilinear multiplication (bracket).
3. $\forall x, y \in L: [x, y] = -[y, x]$ (Skew symmetry)
4. $\forall x, y, z \in L: x \cdot [y, z] + [z, x] \cdot y + [y, x] \cdot z = 0$ (Jacobi identity)

Lie algebras are, in general, non-associative algebras, i.e.

$$[x, [y, z]] 
eq [[x, y], z]$$

$\dim L = n$, $\{e_i\}_{i=1}^n$ is a basis of $L$.

$$[e_i, e_j] = \sum_{k=1}^n c_{ij}^k e_k$$

$c_{ij}^k$ are structural constants.

$\langle \cdot, \cdot \rangle$ is bilinear $\Rightarrow c_{ij}^k$ form a tensor.

$$c_{ij}^k = \alpha_i^t \cdot a_j^s \cdot \alpha_k^r \cdot c_{ts}^k$$

$A$ is matrix of change of basis.

$$A = \Pi \alpha_k \Pi = A^{-1}$$

$L_1 \cong L_2$ if \exists $\psi: L_1 \to L_2$ isomorphism of linear spaces $L_1$ and $L_2$:

$$\forall ([x, y]_1) = [(\psi(x), \psi(y))]_2$$
Examples of Lie algebras:

1) Commutative Lie algebras:
\[ [e_i, e_j] = 0 \text{ for } 1 \leq k, i, j \leq n \text{, i.e. } [e_i, e_j] = 0, 1 \leq i, j \leq n \]
\[ [e_i, e_j] = 0. \]

2) \( R^3 \), \( [\cdot, \cdot] : R^3 \times R^3 \rightarrow R^3 \) vector product
\( e_1, e_2, e_3 \) orthonormal basis with positive orientation
\[ [e_1, e_2] = e_3 \]
\[ [e_2, e_3] = e_1 \]
\[ [e_3, e_1] = e_2 \]

3) A is an associative algebra over field \( K \) (ex: \( L(L) \) algebra of all linear operators)
\[ [x, y] := xy - yx \] commutator

4) A is an algebra (not necessary associative)
\[ D(A) = \{ D \in L(A) | D(xy) = D(x)y + xD(y) \} \]
\[ [D_1, D_2] := D_1 D_2 - D_2 D_1 \in D(A) \]

5) \( M \) is manifold; \( \text{Vect}(M) \) is a set of all smooth vector fields on \( M \)
\[ \text{Vect}(M), [\cdot, \cdot] \text{ is commutator} \]

6) Linear Lie algebras:
\[ \text{GL}(n, \mathbb{C}) \], \( \text{sl}(n, \mathbb{C}) = \{ A \in \text{GL}(n, \mathbb{C}) | \text{tr}A = 0 \} \]
\[ \text{O}(n, \mathbb{C}) = \{ A \in \text{GL}(n, \mathbb{C}) | A + A^* = 0 \} \]
\[ [A; B] := AB - BA \]
1) \( R^3, [\cdot,\cdot] : R^3 \times R^3 \rightarrow R^3 \) is vector product

\[
[e_1; e_2] = e_3 \\
[e_2; e_3] = e_1 \\
[e_3; e_1] = e_2
\]

\( [x; y] = -[y; x] \) \text{ skew symmetric}

2) Th. Jacobi identity: \( \forall x \in R^3, y \in R^3, z \in R^3: \)

\[
[x; [y; z]] + [z; [x; y]] + [y; [z; x]] = 0
\]

3) \( \mathcal{L}(L) \) is an algebra of all linear operators

\( A \in \mathcal{L}(L), \ B \in \mathcal{L}(L) \)

\[
[A; B] := A \cdot B - B \cdot A \quad \text{commutator}
\]

\( [\cdot, \cdot] : \mathcal{L}(L) \times \mathcal{L}(L) \rightarrow \mathcal{L}(L) \)

a) \( [A; B] = -[B; A] \)

b) \( [A; [B; C]] + [C; [A; B]] + [B; [C; A]] = 0 \)

4) \( O(n, C) := \{ A \in \mathcal{L}(L) \mid A = -A^T \} \)

\( \forall A \in O(n, C), B \in O(n, C) : \)

\[
[A; B] = A \cdot B - B \cdot A \in O(n, C)
\]

\( (A; B)^T = (A \cdot B - B \cdot A)^T = (A \cdot B)^T - (B \cdot A)^T = B^T A^T - A^T B^T = \)

\[
= (-B)(-A) - (-A)(-B) = BA - AB = -[A; B]
\]
Introduction to Lie algebras, Lie groups and Lie symmetries.

Heisenberg algebra \( H_1 \)

\[
A \circ B - B \circ A = I
\]

"Schrödinger" representation: \( A = \frac{\partial}{\partial t} : \exp(\rho(x_1, x_2)) \), \( B = M_t : \exp(\rho(x_1, x_2)) \)

OBS! \( A \circ I = I \circ A \), \( B \circ I = I \circ B \) (\( I \) belongs to the center of the algebra \( H_1 \))

Heisenberg Lie algebra (Generalization of \( H_1 \)) \( I \rightarrow C \) ("Central" element)

Associate algebra with three generators \( A, B, C \), and defining Commutation relations:

\[
\begin{align*}
A \circ B - B \circ A &= C \\
A \circ C - C \circ A &= 0 \\
B \circ C - C \circ B &= 0
\end{align*}
\]

If \( C = I \), then we get the Heisenberg algebra \( H_1 \).

More correct terminology:

Universal enveloping (associative) algebra of the Heisenberg Lie algebra with Lie bracket multiplication defined on generators \( A, B \) and \( C \) as:

\[
\begin{align*}
[A, B] &= C \\
[A, C] &= 0 \\
[B, C] &= 0
\end{align*}
\]

OBS! Commutator or bracket product of any two generators is a linear combination of generators:

\[
[A_i, A_j] = \sum_{k=1}^n c_{ij}^k A_k
\]
Commutation rules for functions of generators of Heisenberg Lie algebra. Commutator

\[ AB - BA = C \]
\[ AC - CA = 0 \]
\[ BC - CB = 0 \]

For any polynomial (or power series) function \( f(x) \):

\[ [A, f(B)] = C f'(B) \]
\[ [f(A), B] = C f'(A) \]

where \( f' = \frac{df}{dx} \)

Example: In \( H_n \), \( C = I \) and so \( AB - BA = I \)

\[ [A, f(B)] = f'(B), \quad [f(A), B] = f'(A) \]

For \( f(t) = t^n \), we get \( f'(t) = n t^{n-1} \),

\[ [A, B^n] = n B^{n-1}, \quad [A^n, B] = n A^{n-1} \]

Proof of (*) (main steps):

1) For any \( X, Y \) and \( Z \):

\[ X^n Y - YZ^n = \sum_{j=0}^{n-1} X^{n-1-j} (XY - YX) Z^j \]

2) \[ [A, B^n] = AB^n - B^n A = \sum_{j=0}^{n-1} B^{n-1-j} (AB - BA) B^j = \sum_{j=0}^{n-1} B^{n-1-j} C B^j \]

3) For any polynomial or power series \( f(t) = \sum_{i} \alpha_i t^i \), multiply \( x \) by \( \alpha_d \) and sum up.
Exponential commutation rules
and the Heisenberg Lie group
multiplication laws

\[
\begin{align*}
AB - BA &= C \\
AC - CA &= 0 \\
BC - CB &= 0
\end{align*}
\]

Theorem: For \( \mathbb{R}^3 \), \( t \in \mathbb{R} \):
\[
(e^A)(e^B) = e^{AB} = e^{BA} = (e^B)(e^A) = e^{BA} = e^{AB}
\]

(Proof uses Theorem 1.)
Example: \( C = I \), Heisenberg algebra \( AB - BA = I \).
\[
\begin{align*}
e^{\hat{A}t} e^{\hat{B}t} &= e^{\hat{B}t} e^{\hat{A}t} \\
U(t) V(s) &= e^{\hat{B}t} V(s) U(t) \\
U(t) V(s) &= q(s,t) V(s) U(t)
\end{align*}
\]

Weyl form of Heisenberg canonical commutation relations of Quantum Mechanics.

Observe! \( \{ e^{\hat{A}t} \mid t \in \mathbb{R} \} \) is one-parameter group (thinfinitesimal)
parameter manifold is \( \mathbb{R}^3 \). \( t \in \mathbb{R} \).

Group law for \( q(t) = e^{\hat{A}t} \):
\[
q(t)q(s) = e^{\hat{A}t} e^{\hat{A}s} = e^{\hat{A}(t+s)} = q(t+s)
\]

Group \( \{ e^{\hat{A}t} \mid t \in \mathbb{R} \} \) is commutative \( q(t)q(s) = q(s)q(t) \)

Inverse element: \( q(t)^{-1} = (e^{\hat{A}t})^{-1} = e^{-\hat{A}t} = q(-t) \)

Elements in Heisenberg Lie group:
\[
q(s,t,r) = e^{\hat{B}s} e^{\hat{A}t} e^{\hat{C}r}
\]

Parameter manifold: \( \mathbb{R}^3 \), \( s \in \mathbb{R} \), \( r \in \mathbb{R} \)
Heisenberg Lie group law: \( \) parameters for product
\[
q(s_1,s_2,t_1,t_2,r_1,r_2) = q(s_1+s_2,t_1+t_2,r_1+r_2)
\]
Heisenberg Lie group law:

\[ AB - BA = C, \quad AC - CA = 0, \quad BC - CB = 0. \]

Heisenberg Lie algebra can be also:

\[ e^{tA}, e^{sB}, e^{cC} \]

One-parameter \((IR)\) groups with infinitesimal generators \(A, B\) and \(C\).

General group element of Heisenberg Lie group:

\[ g(s, t, c) = e^{sB} e^{tA} e^{cC} \]

Identity (unit) element:

\[ g(0, 0, 0) = e^{0B} e^{0A} e^{0C} = I \]

The Heisenberg Lie group law:

\[ g(s_1, t_1, c_1) g(s_2, t_2, c_2) = g(s_1 + s_2, t_1 + t_2, c_1 + c_2 + t_1 s_2) \]

Proof: By exponential commutation rules

\[ g(s_1, t_1, c_1) g(s_2, t_2, c_2) = e^{s_1 B} e^{t_1 A} e^{c_1 C} e^{s_2 B} e^{t_2 A} e^{c_2 C} = e^{s_1 B} e^{(t_1 + t_2) A} e^{c_1 C} e^{s_2 B} e^{(t_1 + t_2) A} e^{c_2 C} = e^{(s_1 + s_2) B} e^{(t_1 + t_2) A} e^{(c_1 + c_2 + t_1 s_2) C} = g(s_1 + s_2, t_1 + t_2, c_1 + c_2 + t_1 s_2). \]
General "Leibniz rule"
as a corollary of exponentialcommutation rules.

\[
e^{tA}e^{sB} = e^{sB}e^{tA}e^{stC}
\]

\[
\left(\sum_{j=0}^{\infty} \frac{A^j}{j!} t^j\right)\left(\sum_{k=0}^{\infty} \frac{B^k}{k!} s^k\right) = \left(\sum_{k=0}^{\infty} \frac{B^k}{k!} s^k\right)\left(\sum_{j=0}^{\infty} \frac{A^j}{j!} t^j\right)\left(\sum_{l=0}^{\infty} \frac{C^l}{l!} s^l t^l\right)
\]

Expand and compare coefficientsin front of powers of \(t\) and \(s\).

Theorem 3: (General Leibniz Rule for)
Heisenberg Lie algebra

\[
A^nB^m = \sum_{K=0}^{\min(n,m)} \frac{\min(n,m)!}{K!(n-K)!(m-K)!} A^n B^m C^k
\]

Example: \(C = I\), Heisenberg algebra \(AB-BA=I\)

\[
A^nB^m = \sum_{K=0}^{\min(n,m)} \frac{\min(n,m)!}{K!(n-K)!(m-K)!} A^n B^m C^k
\]

\(A = D_t = \frac{d}{dt}\), \(B = M_t\) \(f(t) \rightarrow tf(t)\)

\(t \rightarrow f(t) \in C^\infty(R)\)

General Leibniz formula

\[
D^n (t^m f(t)) = \sum_{K=0}^{\min(n,m)} \frac{\min(n,m)!}{K!(n-K)!(m-K)!} t^{m-k}D^{n-k} f(t)
\]

\(n = 1:\)

\[
D_t (t^m f(t)) = \left(\frac{m!}{m! (m-1)!}\right) m \uparrow f(t)
\]

(\(m\uparrow\) is the Rising Power Function)
First, the general notion "Lie Group" will be explained. It will be shown that a Lie Group is generated by "infinitesimal transformations", and all representations of the group can be obtained from representations of the infinitesimal "Lie Algebra".

1.8 Lie Groups and their Infinitesimal Transformations

A. Lie Groups

A Lie Group is a group and at the same time an $n$-dimensional manifold, which means that in the neighbourhood of any group element $T_0$ the group elements $T(s)$ are determined by $n$ real parameters $s_1, \ldots, s_n$.

Example. The group $\mathbb{R}_3$ of real rotations in 3 dimensions. Every rotation has a rotation axis $\alpha$ and a rotation angle $\varphi$. By the choice of a unit vector $\hat{\alpha}$ the axis can be directed, and by the corkscrew-rule one direction of rotation can be defined as positive. Now the vector $\varphi \hat{\alpha}$ defines the rotation uniquely, for if $\hat{\alpha}$ is replaced by $-\hat{\alpha}$ and $\varphi$ by $-\varphi$, the rotation remains the same. Hence every rotation $T(s)$ is uniquely determined by the coordinates $s_1, s_2, s_3$ of the vector $\varphi \hat{\alpha}$. Thus $\mathbb{R}_3$ is seen to be a 3-dimensional Lie Group.

Quite generally, let $U$ be a neighbourhood of the unity element $I$ of a Lie Group $G$, and let $T(s)$ be the group element in $U$ corresponding to the parameter values $s_1, \ldots, s_n$. If $T(s)$ and $T(t)$ are sufficiently near to unity, $T(s) T(t)$ and $T(s)^{-1}$ will again lie in $U$, hence we can write

$$T(s) T(t) = T(u),$$

$$T(s)^{-1} = T(v).$$

The parameters $u$ determining the product $T(s) T(t)$ are supposed to be continuous functions of the $s$ and $t$, and the $v$ to be continuous functions of the $s$:

$$u = f(s, t); \quad v = g(s).$$

According to a theorem of Gleason, Montgomery, and Zippin\(^1\), the parametrization can always be chosen in such a way that $f$ and $g$ are analytic functions, i.e. power series. In the case of a one-dimensional Lie Group it is even possible to write the laws of composition as

$$u = s + t; \quad v = -s.$$

Therefore, from now on $I$ shall assume $f$ and $g$ to be analytic functions, and in the one-dimensional case $I$ shall assume

$$T(s) T(t) = T(s + t),$$

$$T(s)^{-1} = T(-s).$$

B. One-dimensional Lie Groups and Semi-Groups

The group of translations along the $t$-axis is isomorphic to the additive group of real numbers. How can we find all representations of this group by linear transformations of a vector space $\mathcal{V}$ into itself? More precisely: How can we find linear transformations $T(s)$ of $\mathcal{V}$ into itself which are continuous functions of $s$ satisfying the conditions

\begin{align}
T(s)T(t) &= T(s+t), \\
T(0) &= I?
\end{align}

If $\mathcal{V}$ is finite-dimensional and if the matrix-valued function $T(s)$ is supposed to have a continuous derivative, the solution is easy. Differentiating (18.1) with respect to $s$ and putting $s = 0$, one obtains

\begin{align}
A \frac{dT}{dt} = \frac{d}{dt} T(t)
\end{align}

where $A$ is the derivative of $T(s)$ at $s = 0$. The solution of this differential equation with the initial condition $T(0) = I$ is

\begin{align}
T(t) &= e^{A} \\
&= 1 + tA + \frac{1}{2!}(tA)^2 + \cdots
\end{align}

This power series converges for all $t$. The linear transformation $A$ is called the infinitesimal transformation generating the one-dimensional Lie Group. If $A$ is a diagonal matrix having diagonal elements $a_1, a_2, \ldots$, the matrix $e^{A}$ has diagonal elements $\exp(ia_1), \exp(ia_2), \ldots$.

If the transformations $T(t)$ are applied to a fixed vector $x_0$, the point

$\begin{align}
x(t) = T(t)x_0
\end{align}$

describes an orbit. From (18.3) we have

$\begin{align}
\frac{dx}{dt} = Ax(t),
\end{align}$

i.e. the velocity at any point $x$ of the orbit is just $Ax$. Thus, the geometrical picture of an infinitesimal transformation $A$ is just the velocity field of a stationary flow. The transformation $T(t)$ is obtained by following the flow during a certain time $t$.

Elie Cartan and John von Neumann showed that the assumption of differentiability of the function $T(t)$ is not necessary; it is a consequence of (18.1) and the assumption of continuity. For a simple proof see van der Waerden\(^1\). Hence we have the theorem:

**Every continuous representation of the one-dimensional translation group by linear transformations of a finite-dimensional vector space $\mathcal{V}$ is generated by an infinitesimal linear transformation $A$ and given by**

\begin{align}
T(t) &= e^{A}
\end{align}

This theorem was generalized to Hilbert spaces by M. H. Stone\(^2\) and to more general vector spaces by E. Hille and K. Yosida\(^3\). Stone proved:

**Suppose the unitary transformation $T(t)$ of a Hilbert space $\mathcal{H}$ is a continuous function of the real variable $t$ satisfying the conditions**

$\begin{align}
T(s)T(t) &= T(s+t), \\
T(0) &= I.
\end{align}$


Then a self-adjoint linear operator $A$ exists, defined by

\[(18.5) \quad Ax = i \lim_{s \to 0} \frac{U(s) - I}{s} x \]

such that

\[(18.6) \quad U(t) = \exp(-itA).\]

Independent of each other, Hille and Yosida proved a still more general theorem. They considered semigroups of bounded linear transformations $T(t)$ of a locally convex vector space $\mathcal{V}$ into itself, where $T(t)$ is a continuous function of $t$, defined for $t \geq 0$ and satisfying the conditions (18.1) and (18.2). Under these conditions they first proved the existence of an infinitesimal operator $A$ defined on an everywhere dense subset of the space $\mathcal{V}$, according to (18.5). If the real part of the complex variable $u$ is sufficiently large, the operator $uI - A$ possesses a bounded inverse

\[(18.7) \quad R(u) = (uI - A)^{-1},\]

which is the Laplace transform of $T(s)$ in the following sense:

\[(18.8) \quad R(u) x = \int_0^\infty e^{-ut} T(s)x \, ds \]

It is well-known that a continuous function $f(t)$ is uniquely determined by its Laplace transform $F(u)$. One can calculate $f(t)$ by means of the well-known Inversion Formula: 

\[(18.9) \quad f(t) = \lim_{M \to \infty} \frac{1}{2\pi i} \int_{-iM}^{iM} e^{ut} f(u) \, du.\]

If $f(t)$ is bounded, this formula holds for every positive $\varepsilon$. It also holds if the values of $f(t)$ are vectors in Hilbert space, the proof is just the same as in the classical case of a real or complex-valued function $f(t)$. Hence (18.8) can be solved for $T(t)x$ by means of the Inversion Formula

\[(18.10) \quad T(t)x = \lim_{M \to \infty} \frac{1}{2\pi i} \int_{-iM}^{iM} e^{uI} R(u)x \, du \]

Another expression for $T(t)$ was given by Hille and Yosida. If $T(t)$ is unitary and hence $A$ self-adjoint, Yosida's formula reduces to Stone's formula (18.6).

\[\text{3 The limit is a strong limit in the sense of Hilbert Space topology.}\]
C. Causality and Translations in Time

Consider a quantum-mechanical system, e.g., an atom or molecule or quantum field, which is isolated from the rest of the world during a certain time $T$. Let the state of the system during a short time from $0 - \delta$ to $0 + \delta$ be given by an element $\phi_0$ of a Hilbert space. The Principle of Causality requires that the state of the system at any later time $t$, or rather between $t - \delta$ and $t + \delta$, is uniquely determined by $\phi_0$ according to a law. It seems reasonable to assume that this law can be expressed by a linear transformation $U(t)$:

$$\Phi(t) = U(t) \phi_0.$$

Finally, we may assume that the transformation $U(t)$ is unitary. In all existing theories, this postulate is always fulfilled.

An immediate consequence of these assumptions is

$$U(s + t) = U(s) U(t)$$

$$U(0) = I.$$

It also seems reasonable to assume that in a very small time the state vector $\phi(t)$ does not change much, which means that $U(t) \phi_0$ is a continuous function of $t$. Hence we suppose that the unitary transformations $U(t)$ form a continuous representation of the semi-group of non-negative translations in time.

To this representation we may apply the theorems of Stone, Hille, and Yosida, and conclude that a self-adjoint linear operator exists, which was formerly denoted by $A$ and which we shall now call $\frac{\hbar}{i} H$, such that

$$(18.11) \quad U(t) = \exp(-i \frac{\hbar}{i} H t).$$

The operator $-i \frac{\hbar}{i} H$ was defined as derivative of $U(s)$ at $s = 0$. Now if we differentiate the equation

$$U(s + t) \phi_0 = U(s) U(t) \phi_0$$

with respect to $s$ and put $s = 0$, we obtain

$$(18.12) \quad \frac{d}{dt} \phi(t) = -i \frac{\hbar}{i} H \phi(t).$$

More precisely: if $\phi_0$ is any state vector for which $H \phi_0$ is defined, $H$ can also be applied to $\phi(t)$, and the differential equation (18.12) holds. It has just the form of the Schrödinger equation, hence we may call $H$ the Hamiltonian or Energy Operator, and we have the theorem:

If a Law of Causality holds, according to the assumptions stated above, a self-adjoint Hamiltonian $H$ exists such that (18.11) and (18.17) hold.

The theorems of Hille and Yosida are not only interesting from a theoretical point of view. They also give us a tool for the practical solution of the Schrödinger equation (18.12) by means of a Laplace Transformation. To explain this, let us re-write the equations (18.7) and (18.8) of Hille and Yosida as

$$(18.13) \quad R(u) \phi_0 = \int_{0}^{\infty} e^{-ut} \phi(t) \, dt.$$ 

and

$$(18.14) \quad R(u) \phi_0 = (u I + i \hbar^{-1} H)^{-1} \phi_0.$$ 

The first formula says: $R(u) \phi_0$ is just the Laplace transform of the function $\phi(t)$. The second formula says that this Laplace transform can be computed from the equation

$$(18.15) \quad (u I + i \hbar^{-1} H) R(u) \phi_0 = \phi_0.$$ 

The formulae (18.14) and (18.15) imply that $R(u) \phi_0$ always belongs to the domain of definition of the operator $H$, no matter how $\phi_0$ may be chosen in Hilbert space, whereas the Schrödinger equation (18.12) has a meaning only if $\phi_0$ belongs to the domain of definition of $H$. Hence, one can always compute $\phi(t)$ by means of its Laplace transform $R(u) \phi_0$, no matter what $\phi_0$ is. To compute $\phi(t)$ one can use, once more, the inversion formula

$$(18.16) \quad \phi(t) = \lim_{M \to \infty} \frac{1}{2 \pi i} \int_{-iM}^{iM} e^{iu} R(u) \phi_0 \, du.$$
D. The Lie Algebra of a Lie Group

From now on, we shall consider only linear transformations in finite-dimensional vector spaces. Let us first recall that for every such transformation \( A \) the series

\[
e^A = 1 + A + \frac{1}{2!} (A)^2 + \cdots
\]

converges, that the transformations \( e^A \) form a one-dimensional Lie Group, and that every one-dimensional Lie Group can thus be obtained from an infinitesimal transformation \( A \).

Quite generally, if an \( n \)-dimensional Lie Group \( G \) consists of linear transformations \( T \), the parameters \( s_1, \ldots, s_n \) in a neighbourhood of \( I \) can be chosen in such a way that the transformations \( T(s) \) are power series in \( s_1, \ldots, s_n \):

\[
T(s) = I + s_1 I_1 + \cdots + s_n I_n + \cdots
\]

Differentiating (18.17) with respect to \( s_1, \ldots, s_n \) and putting \( s = 0 \), one obtains \( n \) infinitesimal transformations \( I_1, \ldots, I_n \). Now all group elements in a neighbourhood \( U \) of \( I \) can be written as

\[
T = \exp(t_1 I_1) \exp(t_2 I_2) \cdots \exp(t_n I_n)
\]

the \( t_1, \ldots, t_n \) being a new set of parameters.

The linear transformations

\[
J = u_1 I_1 + \cdots + u_n I_n
\]

obtained by differentiating (18.17) in the direction of an arbitrary vector \( u \), are called the infinitesimal transformations of the group \( G \). Every group element in a neighbourhood of \( I \) can be written as

\[
T = \exp(u_1 I_1 + \cdots + u_n I_n) = \exp(J)
\]

and hence belongs to a one-dimensional subgroup generated by an infinitesimal transformation \( J \) of \( G \). The \( u \) are called canonical parameters.

The infinitesimal transformations \( J \) defined by (18.19) form an algebra, the Lie Algebra belonging to the group \( G \). In this algebra, three operations are defined:

1. addition
2. multiplication by real numbers
3. the operation \([A, B] = AB - BA\).

The commutator \([A, B]\) is obtained by developing

\[
e^{iA} e^{iB} e^{-iA} e^{-iB}
\]

in a power series and retaining the term with \( i \) only. It follows that the brackets \([A, B]\) always belong to the Lie Algebra. In particular we have

\[
[A, B] = \sum c_{ij}^{\prime} A_i B_j.
\]

The \( c_{ij}^{\prime} \) are called the structural constants of the Lie Algebra. They determine the structure of the group in a neighbourhood \( U \) of \( I \). Two Lie Groups having the same structural constants are locally isomorphic.

Globally they need not be isomorphic.

Example. The infinitesimal transformations \( A_1, A_2, A_3 \) of the three-dimensional rotation group \( \mathbb{SO}_3 \) are just the infinitesimal rotations \( I_1, I_2, I_3 \) about the \( x, y, \) and \( z \)-axis. Their matrices are

\[
I_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad I_2 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{pmatrix}, \quad I_3 = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}
\]

The commutator relations are

\[
\begin{align*}
I_1 I_2 - I_2 I_1 &= I_3 \\
I_2 I_3 - I_3 I_2 &= I_1 \\
I_3 I_1 - I_1 I_3 &= I_2
\end{align*}
\]

Later on we shall see that the group \( \mathbb{SO}_3 \) is locally isomorphic to the group \( SU(2) \) of unitary transformations in 2 dimensions with determinant 1.
E. Representations of Lie Groups

As in Chapter II, we shall denote the elements of a group $\mathcal{G}$ by letters like $a, b, \ldots$ and the representing matrices by the corresponding capital letters $A, B, \ldots$. We consider only continuous representations, which means that the representing matrix $B$ is supposed to be a continuous function of the group element $b$, defined in a neighbourhood $U$ of the unity element $e$. In such a neighbourhood $U$ the elements $b$ may be represented as products (18.18):

\[(18.21) \quad b(t) = \exp(t_1 I_1) \cdots \exp(t_n I_n).\]

Any continuous representation $b \to B$ yields a continuous representation of the one-dimensional subgroup formed by the elements

\[(18.22) \quad b_1(t_1) = \exp(t_1 I_1).\]

Now we have seen that any such representation is generated by an infinitesimal transformation $A_1$, and that the element (18.22) is represented by the matrix

\[B_1(t_1) = \exp(t_1 A_1).\]

The same holds for $b_2(t_2) = \exp(t_2 I_2)$, and so on. Hence the product (18.21) is represented by

\[(18.23) \quad B(t) = \exp(t_1 A_1) \cdots \exp(t_n A_n).\]

This means: the matrix $B(t)$ is an analytic function of $t_1, \ldots, t_n$, and the representation is completely determined by its infinitesimal transformations $A_1, \ldots, A_n$.

The group element

\[\exp(s I_1) \exp(t I_2) \exp(- s I_1) \exp(- t I_2)\]

must be represented by the matrix

\[\exp(s A_1) \exp(t A_2) \exp(- s A_1) \exp(- t A_2).\]

Expanding in power series and comparing the coefficients of $st$, one sees that to $[I_1, I_2]$ corresponds $[A_1, A_2]$, and just so for any commutator $[I_i, I_j]$. Thus we see that the equations

\[[I_i, I_j] = \Sigma c_{ij}^k I_k\]

which hold for the $I_i$, must hold just as well for the $A_i$:

\[(18.24) \quad [A_i, A_j] = \Sigma c_{ij}^k A_k.\]

Thus, the problem to find all continuous representations of $\mathcal{G}$ can be reduced to a much simpler algebraic problem: To find a set of $n$ matrices $A_1, \ldots, A_n$ satisfying the equations (18.24).

Any solution of this algebraic problem leads to a local representation of $\mathcal{G}$, i.e. to a representation of a neighbourhood of $e$ in $\mathcal{G}$, in which products $bc$ are represented by products $BC$. If the representation is extended to the whole group, it is possible that one obtains a multi-valued representation.
Problem: \( \mathfrak{sl}(2) \) denotes the Lie algebra of \( 2 \times 2 \) real matrices of trace zero \((\text{tr} A = a_{11} + a_{22} = 0)\). Let \( \Delta = \begin{pmatrix} 0 & 0 \\ -1 & 0 \end{pmatrix} \), \( R = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \), \( p = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \).

Show that \( \mathfrak{sl}(2) = \left\{ x_1 \Delta + x_2 R + x_3 p : x_1, x_2, x_3 \in \mathbb{R} \right\} \).

a) Show that \( \Delta, R \) and \( p \) satisfy commutation relations
\((\ast)\): \([\Delta, R] = p; \quad [p, R] = 2R; \quad [\Delta, p] = 2\Delta\)
where \([A, B] := AB - BA \) (commutator).

b) Show that the operators on \( C^\infty(\mathbb{R}^2) \) given by
\( \Delta = \frac{1}{x^2} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) \), \( R = \frac{1}{x}(x^2 + y^2) \),
(\text{"Laplacian in } 2\text{ dimensions"})
\( p = x \frac{\partial}{\partial x} + y \frac{\partial}{\partial y} + 1 \)
satisfy commutation relations \((\ast)\).

c) Show that the operators in \( C^\infty(\mathbb{R}^n) \) given by
\( \Delta = \frac{1}{x^2} \sum_{j=1}^{N} \frac{\partial^2}{\partial x_j^2} \), \( R = \frac{1}{x} \sum_{j=1}^{N} x_j^2 \), \( p = \sum_{j=1}^{N} \frac{\partial}{\partial x_j} + \frac{N}{x} \)
(\text{"Laplacian in } \mathbb{R}^n\text{ dimensions"})
satisfy commutation relations \((\ast)\).

Groups, representations, Symmetries, Equations of Applications.

Let $\mathcal{G}$ be any group and let the elements $a$ of $\mathcal{G}$ be mapped upon linear transformations $A$ of a vector space $\mathcal{V}$ or, what amounts to the same thing, upon matrices $A$, such that the map of $ab$ is $AB$. Such homomorphisms are called representations $\rho$ of $\mathcal{G}$ by linear transformations or by matrices. The dimension $n$ of the space $\mathcal{V}$ is called the degree of the representation $\rho$.

The application of the theory of Group Representations to Quantum Mechanics is based upon the following idea.

Schrödinger's differential equation

$$H\psi = E\psi$$

is invariant with respect to certain transformations of the variables $x, y, z, \ldots$, such as

1. permutations of the coordinates of electrons and of equal nuclei,

2. translations, rotations and reflections, which leave unchanged the field of force and hence the Hamiltonian $H$. Let us consider a few special cases of 2.

2a. If we have an atom, in which the nucleus is regarded as fixed, we have to consider the reflections and rotations leaving invariant this point.

2b. If the atom is placed in a homogeneous electric or magnetic field, the group of rotations about a fixed point must be replaced by the group of rotations about a fixed axis. There are also reflections which leave the field invariant.

2c. If we have a two-atom molecule, and if we consider (in a first approximation) the nuclei as being fixed in space, the rotations to be considered are rotations about the line connecting the nuclei, and the reflections are with respect to the planes passing through this line. If the two nuclei have equal atomic numbers and hence equal charges, we may also consider the reflection with respect to a plane perpendicular to the axis, which interchanges the two nuclei.

The permutations, rotations etc. just considered, which leave invariant the Hamiltonian $H$, always form a group $\mathcal{G}$. For if the
transformations \( A \) and \( B \) leave \( H \) invariant, so does \( AB \), and so does \( A^{-1} \). The identity \( I \) trivially leaves \( H \) invariant.

The transformations of this group can be applied to the wave function \( \psi \), as follows. Let \( q_1, \ldots, q_f \) be the coordinates of the \( f \) electrons of the atom or molecule under consideration, the single letter \( q \) standing for a triple of three coordinates \( x, y, z \). If a spatial transformation \( T \) transforms the points \( q_1, \ldots, q_f \) into points \( q'_1, \ldots, q'_f \), the transformed wave function \( \psi' = T\psi \) will be defined (as in \( \S 8 \)) by the formula

\[
\psi'(q'_1, \ldots, q'_f) = \psi(q_1, \ldots, q_f)
\]

or, what amounts to the same thing, by

\[
\psi'(q_1, \ldots, q_f) = \psi(T^{-1}q_1, \ldots, T^{-1}q_f).
\]

It is easy to see that this transformation of functions is a linear transformation:

\[
(\psi + \psi')' = \psi' + \psi',
\]

\[
(c\psi)' = c\psi'.
\]

If two transformations \( S \) and \( T \) are applied one after the other (first \( T \), next \( S \)), we have

\[
(St)\psi = S(T\psi).
\]

Since these transformations leave invariant Schrödinger's differential equation, they transform solutions \( \psi \) into solutions \( \psi' \) belonging to the same energy value. Hence:

The eigenfunctions of any given energy level are linearly transformed by the group \( \mathcal{G} \), and these transformations form a representation of the group \( \mathcal{G} \).

If we succeed in classifying all possible representations of the groups in question, this will give us at the same time a classification of the eigenfunctions and energy levels of the atoms and molecules. This classification forms, as we shall see, the theoretical basis of spectroscopy.
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Since these transformations leave invariant Schrödinger's differential equation, they transform solutions $\psi$ into solutions $\psi'$ belonging to the same energy value. Hence:

The eigenfunctions of any given energy level are linearly transformed by the group $G$, and these transformations form a representation of the group $G$.

If we succeed in classifying all possible representations of the groups in question, this will give us at the same time a classification of the eigenfunctions and energy levels of the atoms and molecules. This classification forms, as we shall see, the theoretical basis of spectroscopy.