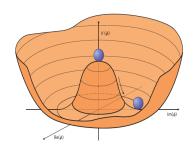
Introduction to Quantum Field Theory using Canonical Quantization

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Web: Course Website

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CHAPTER 1

WHY?

Particles dance on invisible strings,
Fields hum softly, where the vacuum sings.
Ripples of quanta, fleeting and slight,
Woven in spacetime, beyond human sight.
Electrons waver, photons play,
Fields of the cosmos in endless ballet.
Gluons and quarks in a boundless thrall,
The quantum whispers that govern it all.
A silent symphony, unseen, untamed,

- K.A.Rousan

1.1 INTRODUCTION

Wave-particle duality tells us that electrons and photons are more alike than they seem. Even though electrons have mass and charge while photons don't, both can act like waves (think Naruto's Rasengan swirl) and hit like particles (One Punch Man style!). But in classical physics, they're treated differently: electrons and other matter particles are seen as the building blocks of nature, while light is considered as a derived concept, i.e., ripple in the electromagnetic field.

If we want to truly level the playing field between photons and particles, how do we reconcile these differences in the quantum realm? Should we think of particles as the true stars of the show, with the electromagnetic field arising only in some classical limit from a collection of quantum photons? or should we flip the script and see fields as the main characters, with the photon appearing only when we correctly treat the field in a manner consistent with quantum theory?

If the latter is true, we should probably introduce something like an "electron field," whose ripples create electrons with mass and charge—like how Goku charges up his energy field before launching an attack. But why didn't the previous generation of physicists introduce this idea of matter fields, like they did with the electromagnetic field?, what will be the consequences if the last statements were to be true?

In this course, we'll answer these questions. Spoiler alert: the second viewpoint is the best. Fields are the real MVPs, and particles only show up after we quantize these fields. We'll learn how photons emerge from the quantization of the electromagnetic field, and how particles like electrons come from quantizing matter fields. As we dive deeper, we'll also need to introduce fields for quarks, neutrinos, gluons, W and Z bosons, the Higgs, and more. Essentially, there's a field for every fundamental particle in nature, like how every anime has its unique power system (chakra, nen, ki, devil fruits—you get the idea).

Before going any further let's first discuss the units and symbols we are going to use.

1.1.1 Units

In nature we have 3 – fundamental dimensionful constants c = speed of light, \hbar =reduced planck's constant and G = newton's constant. They have dimensions as follows:

Name	Value in SI	Units
c	2.99792458	$ m LT^{-1}$
\hbar	$1.05457182 \times 10^{-34}$ J-s	$L^2 \mathrm{MT}^{-1}$
G	$6.67430 \times 10^{-11} \mathrm{Nm^2/kg^2}$	$L^3M^{-1}T^{-2}$

HIGH ENERGY PHYSICS, we most of the time works with "Natural Units" defined by,

$$c = \hbar = 1 \tag{1.1}$$

This let us express all the dimensionful quantities in terms of s single scale which we most of the time choose as **mass** or **energy** $(E = mc^2 = m)$. The most common choice of m or E is eV.

In terms of the unit we can write,

$$[M] = [E] = [T]^{-1} = [L]^{-1}$$
(1.2)

So, in our unit we can write $m_e \approx 0.5$ MeV. This is in energy's unit. To convert into length's or time, we need to insert the relevant powers of c and \hbar . For example, the length scale λ associated to mass m is the compton wavelength,

$$\lambda = \frac{\hbar}{\text{mc}} \tag{1.3}$$

With this, the electron mass $m_e \approx 0.5 \text{MeV}$ becomes, $m_e \approx 0.5 \text{MeV} = 7.8 \times 10^{20} \text{s}^{-1} = 2.6 \times 10^{10} \text{cm}^{-1}$.

1.1.2 Notation

As we are going to do QUANTUM FIELD THEORY, all our physics are going to unfold on the *Minkowski Space*, flat spacetime. Here all points of space-time are labeled by 4-coordinates. We write these coordinates as,

$$x^{\mu} = (x^{0}, x^{1}, x^{2}, x^{3}) = (t, \vec{x}) = \begin{pmatrix} x^{0} \\ x^{1} \\ x^{2} \\ x^{3} \end{pmatrix}$$
 (1.4)

Similarly, the momentum 4-vector will be written as,

$$p^{\mu} = (p^0, \vec{p})$$

In our case the metric tensor $\eta_{\mu\nu}$ is taken as,

$$\eta_{\mu\nu} = \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & -1 & 0 & 0 \\
0 & 0 & -1 & 0 \\
0 & 0 & 0 & -1
\end{pmatrix}$$
(1.5)

This is mostly negative (+---) sign convention. Using this we can define something known as covariant 4-position vector (this is a very bad thing to say. The vectors are actually just vectors. Their components are called covariant or contra-variant depending upon their transformation rules) as.

$$x_{\mu} = (x_0, x_1, x_2, x_3) = \eta_{\mu \nu} x^{\nu} = (x^0, -x^1, -x^2, -x^3) = (x_0 \ x_1 \ x_2 \ x_3)$$

$$(1.6)$$

In a similar the contravariant x^{μ} can be written as,

$$x^{\mu} = \eta^{\mu\nu} x_{\nu} \tag{1.7}$$

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where $\eta^{\mu\nu}$ is the inverse of the $\eta_{\mu\nu}$, i.e.,

$$\eta_{\mu\nu}\eta^{\nu\sigma} = \delta_{\mu}^{\sigma} \tag{1.8}$$

with

$$\delta_{\mu}^{\sigma} = \begin{cases} 1, & \text{if } \mu = \sigma \\ 0, & \text{if } \mu \neq \sigma \end{cases}$$
 (1.9)

We can also define the inner product between two 4-vectors as,

$$a \cdot b \equiv a^{\mu}b_{\mu} = a_{\mu}b^{\mu} = \eta_{\mu\nu}a^{\mu}b^{\nu} = a^{0}b^{0} - a^{1}b^{1} - a^{2}b^{2} - a^{3}b^{3}$$

$$(1.10)$$

For a 4-vector a^{μ} , we can classify it into 3 catagory depending on it's length $a^2 = a^{\mu}a_{\mu}$,

$$a^{\mu} \text{ is called} = \begin{cases} \text{spacelike if } a^2 < 0 \\ \text{timelike if } a^2 > 0 \\ \text{null or lightlike if } a^2 = 0 \end{cases}$$

In a similar manner, we can define differential operator ∂_{μ} , as

$$\partial_{\mu} = \frac{\partial}{\partial x^{\mu}} = \left(\frac{\partial}{\partial x^{0}}, \frac{\partial}{\partial x^{i}}\right) = \left(\frac{\partial}{\partial t}, \nabla\right)$$

$$\tag{1.11}$$

In 3d, we have seen Laplace operator ∇^2 , we will define another one similar to this in space-time, which is called **d'Alembert operator**,

$$\Box^2 = \partial^2 = \partial^\mu \partial_\mu = (\partial_0)^2 - \nabla^2 \tag{1.12}$$

We all know what is a *Lorentz Transformation*, now we can write the transofrmation formulas in a very compact way!

Let's say we have two frames S and S', where S' is moving relative to S with a velocity $\beta = \frac{v}{c} = v$ along x-axis. Then, we can write the transformation matrix as,

$$\Lambda = \begin{pmatrix}
\gamma & -\beta\gamma & 0 & 0 \\
-\beta\gamma & \gamma & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1
\end{pmatrix}$$
(1.13)

Then, the position 4-vector in S' frame can be written as,

$$x^{\prime \mu} = \Lambda_{\mu}^{\mu} x^{\nu} \equiv \Lambda x \tag{1.14}$$

The dot product of any two 4-vector is invariant under lorentz transformation. This means $a_{\text{new}} \cdot b_{\text{new}} = \mathbf{a} \cdot \mathbf{b}$, i.e., $\Lambda a \cdot \Lambda b = a \cdot b$.

This **Lorentz Transformations form a group**. This group has a name O(3,1). To truely understand the subject, as a result we need the knowledge of group theory(Lie Group). We will discuss that in our course.

1.2 WHY QUANTUM FIELD THEORY?

In classical physics, the primary reason for introducing the concept of the field is to construct laws of Nature that are local. The old laws of Coulomb and Newton involve "action at a distance". This means that force felt by an electron (or planet or maybe you and your crush(if he/she exist)) changes immediately if a distance proton (or star or you) moves. This situation is philosophically unsatisfactory. More importantly, it also expreimentally wrong. The field theories of Maxwell and Einstein remedy the situation, with all interactions mediated in a local fashion by the field

The requirement of locality remains a strong motivation for studying field theories in the quantum world. There are many more reasons for using field theory. Let's see some of them.

1.2.1 Combination of Quantum Mechanics and Special Relativity, Nonconservation of particle number

Consider a particle of mass m trapped in a box of size L. Heisenberg tells us that the uncertainty in the momentum is $\Delta p \geqslant \hbar/L$. In a relativistic setting, momentum and energy are on an equal footing, so we should also have an uncertainty in the energy of order $\Delta E \geqslant \hbar c/L$. However, when the uncertainty in the energy exceeds $\Delta E = 2\text{mc}^2$, then we cross the barrier to pop particle antiparticle pairs out of vacuum. So, particle-antiparticle pairs are expected to be important when a particle of mass m is localized within a distance of order $\lambda = \hbar/\text{mc}$.

At distances shorter than λ , there is a high probability that we will detect particle-antiparticle pairs swarming around the original particle that we put in. The distance λ is called Compton Wavelength. It is always smaller than the de-Broglie Wavelength $\lambda_{\rm dB}=h/|p|$. de-Broglie wavelength is the distance at which the wavelike nature of particle becomes apparent; the Compton wavelength is the distance at which the concept of a single particle breaks down completely^{1,1}.

The necessity of having a multiparticle theory implied by addition of special relativity also can be seen in less obvious way from the consideration of *Causality*. Let's see how!

Consider a free, spin-zero particle of mass m travelling from $\vec{x}_i(\text{at } t=0)$ to $\vec{x}(\text{at } t=t)$. Then, the probability amplitude for this is,

$$A(t) = \langle \vec{x} | e^{-iHt} | \vec{x}_i \rangle \tag{1.15}$$

Here $H = (\vec{p} \cdot \vec{p})/2m = p^2/2m$ is the hamiltonian of the free particle, then

$$A(t) = \langle \vec{x} | e^{-iHt} | \vec{x}_i \rangle$$

$$= \langle \vec{x} | e^{-ip^2t/2m} | \vec{x}_i \rangle$$

$$= \langle \vec{x} | \int \frac{d^3p}{(2\pi)^3} | \vec{p} \rangle \langle \vec{p} | e^{-iHt} | \vec{x}_i \rangle$$

$$= \frac{1}{(2\pi)^3} \int d^3p e^{-itp^2/2m} \langle \vec{x} | \vec{p} \rangle \langle \vec{p} | \vec{x}_i \rangle$$

$$= \frac{1}{(2\pi)^3} \int d^3p e^{-itp^2/2m} e^{i\vec{x} \cdot \vec{p}} e^{-i\vec{p} \cdot \vec{x}_i}$$

$$= \left(\frac{m}{2\pi it}\right)^{3/2} \exp(i \cdot m(\vec{x} - \vec{x}_i)^2 / 2t)$$

$$(1.16)$$

WTF! This expression is non-zero for all \vec{x} and t, impliying that a particle can propagate between any two points in an arbitrarily short time. In a relativistic theory, this would implies a violation of causality.

You may think the problem is the fact that we have used $H = p^2/2m$. Maybe if we use $H = \sqrt{\vec{p} \cdot \vec{p} + m^2}$, we will get correct value? Let's see!(use $\vec{r} = \vec{x} - \vec{x}_i$)

$$A(t) = \langle \vec{x} | \exp\left(-it\sqrt{p^2 + m^2}\right) | \vec{x}_i \rangle$$

$$= \frac{1}{(2\pi)^3} \int d^3p \exp\left(-it\sqrt{p^2 + m^2}\right) \exp\left(i\vec{p} \cdot (\vec{x} - \vec{x}_i)\right)$$

$$= \frac{1}{(2\pi)^3} \int_0^\infty dp \, p^2 \exp\left(-it\sqrt{p^2 + m^2}\right) \int_0^\pi d\theta \sin\left(\theta\right) \exp(i\operatorname{pr}\cos(\theta)) \int_0^{2\pi} d\phi$$

$$= \frac{1}{(2\pi)^2} \int_0^\infty dp \, p \exp\left(-it\sqrt{p^2 + m^2}\right) \frac{(e^{i\operatorname{pr}} - e^{-i\operatorname{pr}})}{i\operatorname{r}}$$

$$= \frac{-i}{(2\pi)^2 r} \int_{-\infty}^\infty dp \, p \exp(i\operatorname{pr}) \exp\left(-iw_p t\right) \quad \text{where } w_p = \sqrt{p^2 + m^2}$$

$$(1.17)$$

^{1.1.} The presence of a multitude of particles and anti-particles at short distance tells us that any attempt to write down a relativistic version of the one-particle schrodinger equation is doomed to failure. There is no mechanism in standard non-relativistic qm to deal with changes in the particle number.

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This integral is quite hard(thet's what ... sorry no joke), it's full of oscillation. It's difficult to tell if it vanishes outside of the light one, i.e., if it vanishes when $(\vec{x} - \vec{x}_i)^2 < 0$ or not. Remember in our natural unit, the speed of light is 1. Since we started with $r = 0(\vec{x}_i)$ at t = 0, if the particle is travelling faster than light, the probability amplitude for r > t will be non-zero.

To do this integration we will use contour integration. We extend p to complex plain and let $p=p_1+ip_2$. We will take the $p_1=\mathrm{Re}(p)$ axis as part of a contour C, and close the contour with a large semicircular arc above or below the p_1 axis. Our integrand is not an analytic function of p(blue part) because the function $w_p=\sqrt{p^2+m^2}$ has branch points at $p=\pm im$. We will choose the branch cuts from im upto $+\infty$ along the $+p_2$ axis and another cut from -im to negative $-\infty$.

We will now distport the semicircular contour C to avoid branch cuts, so that the integrand is an analytic function within the region bounded by the distorted contour as shown in Fig-1.1.

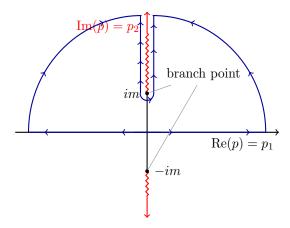


Figure 1.1. Contour for integral of eqn-1.17

The integrand is now analytic within C. Hence, it's zero. We have,

$$A(t) = \frac{i}{(2\pi)^2 r} \left[\int_{\infty}^{m} dp_2 \, p_2 e^{-rp_2 - \sqrt{p_2^2 - m^2} t} + \int_{m}^{\infty} dp_2 \, p_2 e^{-rp_2 + \sqrt{p_2^2 - m^2} t} \right]$$
Changing the limits in 1st term,
$$= \frac{i}{(2\pi)^2 r} \int_{m}^{\infty} dp_2 \, p_2 \, e^{-rp_2} \left[e^{\sqrt{p_2^2 - m^2} t} - e^{-\sqrt{p_2^2 - m^2} t} \right]$$

$$= \frac{i}{2\pi^2 r} \int_{m}^{\infty} dp_2 \, p_2 \, e^{-rp_2} \sinh\left(\sqrt{p_2^2 - m^2} t\right)$$
(1.18)

This is positive. We can more clearly see this by replacing $\sqrt{p_2^2 - m^2}$ by p_2 . This gives us an overestimate,

$$A(t) < \frac{i}{2\pi^2 r} \int_m^{\infty} dp_2 \, p_2 \, e^{-(r-t)p_2}$$

$$< e^{-(r-t)m} \left(\frac{1}{(r-t)^2} + \frac{m}{(r-t)} \right)$$
(1.19)

The chance that the particle is found outside of the forward light cone falls off exponentially as we get farther from the light cone. It's not so bad, it's exponentially damped, and if we go a few factors of 1/m, a few of the particle's compton wavelengths away from the light cone^{1,2}.

QFT actually correct this in a really creative way. We will find that, in the Multiparticle Field Theory, the propagation of a particle across a spacetime interval is indistinguishable from the propagation of an antiparticle in the opposite direction (see Fig-1.2).

^{1.2.} See class note for finding another expression of $A(t) \sim e^{-m(x^2-t^2)^{1/2}}$. For that we need to use Modified Bessel Function. That shows a very interesting phenomenon similar to tunnling but on the surface of light cone. The exact form is $\frac{i \operatorname{tm}^2}{2\pi^2(r^2-t^2)}K_2\Big(m\sqrt{r^2-t^2}\Big)$. For $r\gg t$, $K_2(z)\sim e^{-z}$

When we ask whether an observation made at point \vec{x}_0 can affect an observation made at point \vec{x} , we will find that the amplitudes for particle and antiparticle propagation exactly cancel - so causality is preserved. We will see this later in detail.

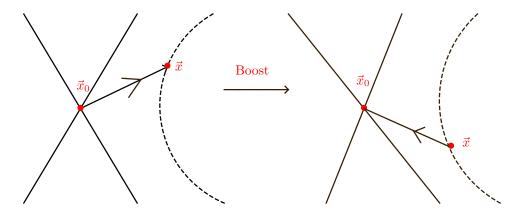


Figure 1.2. Propagation from \vec{x}_0 to \vec{x} in 1-frame looks like propagation from \vec{x} to \vec{x}_0 in another frame.

1.2.2 Same Same not different!

(stop thinking about the song!) "Same particles of same type"

Am I crazy?, wtf is this heading!

This may sound dumb but it's not! What it means is that 2 electrons are identical in every way, regardless of where they came from and what they've been through. The same is true of every other fundamental particle.

For an example, suppose we capture a proton from a cosmic ray which we identify as coming from a supernova lying 8 billion lightyears away. We compare this proton with one freshly minted in a particle accelerator here on earth. The two are exactly the same! How is this possible?, Why aren't there errors in proton production? How can two objects, manufactured so far apart in space and time, be identical in all respects?

One explanation that might be offered is that there's a sea of proton "stuff" filling the universe and when we make a proton we somehow dip our hand into this stuff and from it mould a proton. Then, it's not surprising that protons produced in different parts of the universes are identical. The "stuff" is the proton field (actually they are quark field).

This is not all. In QFT even spins will naturally emerge. We don't even have to put those by hand like we normally do in QFT.

1.3 CONSEQUENCES OF QFT

Quantum field theory has a number of important consequences, both conceptual and experimental. Some of them are:

- Indistinguishable particles: QFT explains the deep fact that "all electrons are the same".

 The particles associated with a field are indistinguishable since they are just excitations of the same underlying field.
- Quantum statistics: Particles with even spin are bosons, those with odd spin are fermions.
 According to the spin-statistics theorem, the physical state of a system is even (odd) under
 the exchange of identical bosons (fermions). In QFT, this fact will emerge as a natural
 consequence of the formalism.

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• Antiparticles: For every particle in Nature there exists a corresponding antiparticle. In QFT, these antiparticles must be added in order for the theory to respect causality.

- Particle creation and destruction: In QFT, particles can be created, annihilated, and
 change their identity. The probabilities for these processes to occur are derived from the
 dynamics of the corresponding quantum fields and especially depend on the nonlinear
 interactions between the fields.
- Forces from particle exchange: Classical waves with nonlinear interactions can scatter from each other. In QFT, this scattering is mediated by the exchange of intermediate particles often called virtual particles.

As these examples show, fundamental features of the physical world are explained by quantum field theory. At a more practical level, it also just works. Some of the most precise predictions in the history of physics were made using quantum field theory.

For example, *QFT predicts an anamalous magnetic dipole moment for muon*. This prediction agrees with experiment at an incredible level of precision:

$$(g_{\mu} - 2)_{\text{theory}} = 0.00233183478(308)$$

 $(g_{\mu} - 2)_{\text{expn.}} = 0.00233184600(168)$

This is just one of many predictions of QFT that have been confirmed by experiment.

QFT is the theoretical foundation of many areas of physics. A few examples are:

- Particle physics: The Standard Model (SM) of particle physics, which accounts for all observed phenomena on length scales larger than 10⁻¹⁸ meters, is a quantum field theory. In this course, we will lay the conceptual foundations for the physics of the SM.
- Condensed matter physics: Although in this course we will deal exclusively with relativistic field theories, QFT has also found important applications to non-relativistic theories such as those found in condensed matter systems. Sound waves in metals and crystals, Fermi liquids of weakly interacting electrons, fluids and superfluids, the behavior of systems near phase transitions, etc. are all described by QFTs.
- Cosmology: There is growing evidence that the early universe went through a period of inflationary expansion. During inflation, the rapid expansion of the spacetime amplified the fluctuations in certain quantum fields, such as the inflaton field and the metric tensor. These fluctuations are believed to be the seeds for the large-scale structure of the universe. Computing this effect is a beautiful application of QFT in curved spacetime.
- **Black holes**: The quantization of fields near the horizon of black holes (BHs) leads to interesting new effects. Hawking famously showed, using QFT in the curved BH background, that BHs aren't truly black, but radiate quantum mechanically.
- General relativity: At long distances, even general relativity (GR) can be described as an effective QFT, namely that of a massless spin-2 particle (the graviton) interacting with the degrees of freedom of the SM.
- String theory: At long distances, string theory also reduces to an e-lective QFT, namely supergravity. At short distances, the extended nature of the string becomes important and a point particle description breaks down.
- *Mathematics*: QFT has also proven to be a source of inspiration for mathematicians. For example, certain QFTs lead to the definition of novel topological invariants including various knot invariants and invariants for higher-dimensional manifolds.

1.4 Assignment-1

I hope you all get a idea of why we should learn QFT and what it can do. In this course we will dive in the realm of QFT and see it's wonders. To be more precise we will also learn Lie Groups as the part of the course. After learning Lie Groups, we will finally start field theory.

Before ending let me write few values which we may need in future:

Quantity	Mass	Length
Observable Universe	10^{-33}eV	$10^{37}m$
Cosmological Constant(Λ)	10^{-3}eV	$10^{-3}m$
$Neutrinos(\nu)$	1eV	$10^{-6}m$
Electron(e)	511keV	$10^{-12}m$
$Muon(\mu)$	106Mev	$10^{-14}m$
Charm $Quark(c)$	1.3 GeV	$10^{-15}m$
$Tau(\tau)$	1.8Gev	$10^{-15}m$
Bottom $Quark(b)$	4.6 GeV	$10^{-16}m$
Higgs $Boson(h)$	125 GeV	$10^{-17}m$
Top $Quark(t)$	175 GeV	$10^{-17}m$
Electroweak $Scale(v)$	250 GeV	$10^{-17}m$
LHC Energy	14TeV	$10^{-18}m$
Planck $Scale(M_{pl})$	10^{18}GeV	$10^{-34}m$

Table 1.1. Some Useful values

One think I should mention: The class note and these notes will be a bit different. For best results follow both.

1.4 Assignment-1

1.4.1 Finding the Lorentz Transformation

- 1. Using the Lorentz Tranformation matrix given in the notes(eqn-1.13), Find the Lorentz Transformation relations normally written in books.
- 2. Let's say we have 3 frames S, S', and S''. S is at rest, S' is moving with velocity β_1 compared to S and S'' is moving with velocity β_2 compared to S'. Find the transformation matrix between S and S''. What conclusion can you give after seeing your final answer?
- 3. As we know in any Lorentz Transformation $x^{\mu} \to x'^{\mu} = \Lambda^{\mu}_{\nu} x^{\nu}$ such that

$$\eta_{\mu\nu}x^{\mu}x^{\nu} = \eta_{\mu\nu}x'^{\mu}x'^{\nu}$$

where $\eta_{\mu\nu}$ is the Minkowski Metric. Show that

$$\eta_{\mu\nu} = \eta_{\sigma\tau} \Lambda_{\mu}^{\sigma} \Lambda_{\nu}^{\tau} \tag{1.20}$$

1.4.2 Natural Units

The photon number density is given by,

$$n_{\gamma} = \frac{2\zeta(3)T^3}{\pi^2} \tag{1.21}$$

Where $\zeta(3)$ is the zeta-function. This expression is found after using the natural unit of $k_B=1$, c=1 and $\hbar=1$. As we know CMB photon temperature is T=2.725K or in eV it is $T=\frac{2.725}{11606} \text{eV}$.

Using these values we found,

Wolfram-lang plugin

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```
In[1]:= T = 2.727/11606  
    0.000234965  
In[1]:= nGamma = (2*Zeta[3]/Pi^2)*T^3  
    3.1598247194119996`10^-12  
    \frac{2T^3\zeta(3)}{\pi^2}
```

The density found is Number/Volume. As we have found it in natural unit it is in eV³. Convert this in cm⁻³. The answer is actually a classic result.

Hint: Try to understand what does c=1 and h=1 actually represent.

1.4.3 Green Function or Propagator

The Green Function $(G(x_2, x_1))$ or Propagator is the amplitude of the particle to go from \vec{x}_1 to \vec{x}_2 point. So,

$$G(\vec{x}_2, t_2; \vec{x}_1, t_1) = \langle \vec{x}_2, t_2 | \vec{x}_1, t_1 \rangle = \langle \vec{x}_2 | \exp(-iH(t_2 - t_1)) | \vec{x}_1 \rangle$$
(1.22)

In our class $t_1 = 0$ and $t_2 = t$. Also, $x_2 = x$ and $x_1 = x_i$.

1. Show that

$$\lim_{t_1 \to t_2} G(\vec{x}_2, t_2; \vec{x}_1, t_1) = \delta^3(\vec{x}_2 - \vec{x}_1)$$
(1.23)

Can you give a physical significance of the result?

2. The propagator must also satisfy a stringent composition law(Transitivity Condition) given as,

$$G(\vec{x}_2, t_2; \vec{x}_1, t_1) = \int d^3 \mathbf{x} G(\vec{x}_2, t_2; \vec{x}, t) G(\vec{x}, t; \vec{x}_1, t_1)$$
(1.24)

Verify this result for

$$G(\vec{x}_2, t_2; \vec{x}_1, t_1) = \left(\frac{m}{2\pi i (t_2 - t_1)}\right)^{3/2} \exp\left(\frac{i m r^2}{2(t_2 - t_1)}\right)$$
(1.25)

with $r^2 = |\vec{x}_2 - \vec{x}_1|^2$ and $t_2 > t_1$.

It should be noted that Transitivity only holds for single particle systems. It doesn't holds for multiparticle system, hence doesn't hold in relativistic Propagator. (Optional but can you show this?)

3. Do the contour integration step by step given in note(**optional**). Note: Actually the amplitude is exponentially decreasing for $r \gg t$ as discussed in class. This is actually very similar to tunneling but on the boundary of light-cone.

Date of Submission: 19th- September 2024.

Also, Give a read to Michael E. Peskin's QFT book chapter - 2 first 3 pages.

CHAPTER 2

LIE GROUPS AND LIE ALGEBRA

In quantum realms, where symmetries glow,

Group theory guides how particles dance and flow.

SU(2) spins, with Pauli in tow,

Defining the paths where fermions go.

Lie algebra forms the Standard frame,

Forces and particles play their game.

Rotations and commutators, all in sync,

Nature's deep structure, on the edge of the brink.

Through symmetry's lens, we glimpse the grand,

The quantum and cosmos, hand in hand.

— K.A.Rousan

2.1 INTRODUCTION

What are Groups? Why do we need them? I mean, we study groups and all of us have some introduction to groups before I suppose. Why we do that?

The answer is very simple. Groups represent symmetry operations. As nature itself contains symmetry, we can actually understand it's working just by using the knowledge of group theory.

In this part, first I will recap few concepts of groups (will not go in detail) then we will go into lie groups.

Also, if possible download and install "SageMath" as we will use these two to write some codes to do some calculations.

If you guys want, you can also download and install "Wolfram Engine" and "WLJS" but i thought about promoting a way to freely use mathematica without installing crack version.

With this all, let's start:

2.1.1 What are Groups?

What is a Group?, Let's start with the definition.

A *Group* implies a map of form $S \times S \to S$, i.e., a binary operation of the elements of the set S. Let us denote the operation by the symbol " \circ ". Then,

$ig({ m Definition} \,\, { m 2.1: \,\, Group} ig)$

A Group (G, \circ) , is a non-empty set G with a binary operator defined to every (ordered) pair of elements with the following rules:

1. For any two elements g_1 and g_2 in a group, a product is defined in G satisfying

$$g_1g_2 = g_1 \circ g_2 = g_3 \in G$$
, $\forall g_1, g_2, g_3 \in G$ (2.1)

2. The group product is associative so that

$$(g_1 \circ g_2) \circ g_3 = g_1 \circ (g_2 \circ g_3) (\equiv g_1 g_2 g_3), \forall g_1, g_2, g_3 \in G$$
 (2.2)

3. The group has a unique *identity element* $e \in G$ such that

$$e \circ g_1 = g_1 \circ e = g_1, \forall g_1 \in G \tag{2.3}$$

4. Any element $g_1 \in G$ has a *unique inverse* element $g_1^{-1} \in G$ so that,

$$g_1 \circ g_1^{-1} = g_1^{-1} \circ g_1 = e$$
 (2.4)

Any set of elements G satisfying all the axioms 2.1, 2.2,2.3 and 2.4 is defined to be a group.

A set of elements which satisfies only the first three axioms, i.e., 2.1, 2.2 and 2.3 but not 2.4 then, it's called **Semi-Group** (Actually only first two axioms are needed but as one can always add the identity elements to the group since one can always add the identity element to the group since its presence, when an inverse is not defined element, is inconsequential and we will adopt this definition commonly used in physics).

Let G be a group. Then for $g_1 \in G$ and $n \in \mathbb{Z}$, we define $g_1^n = g_1 \cdots g_1(n \text{ times})$. Also, I will use $g_1 \circ g_2 = g_1 g_2$.

There are few things we should remeber:

- 1. In general, $g_1g_2 \neq g_2g_1$ but if $g_1g_2 = g_2g_1$, then the group is called **Abelian Group**.
- 2. If $g_1, g_2, \dots, g_n \in G$, then $(g_1g_2 \dots g_{n-1}g_n)^{-1} = g_n^{-1}g_{n-1}^{-1} \dots g_2^{-1}g_1^{-1}$

From the defination, we can say a group is a multiplication table specifying $g_1g_2 \forall g_1, g_2 \in G$. If elements are discrete, we can write the multiplication table in the form,

	e	g_1	g_2	
e	e	g_1	g_2	:
g_1	g_1	g_1g_1	g_1g_2	:
g_2	g_2	$g_{2}g_{1}$	$g_{2}g_{2}$	
:	•••	:	:	• •

Table 2.1. Multiplication Table for some group G

Example 2.1. Let's say we have a group of two elements $S = \{1, -1\}$. Let's say the binary operation is "arithmetic product". In this case, all 4 axioms are satisfied.

If the operation is "arithmetic addition", then 0 which is the identity doesn't exist in the set. As a result, under "addition" S doesn't form a group. Can you say if it's abelian or not?

This group is equivalent of just reflection or maybe flipping a coin.

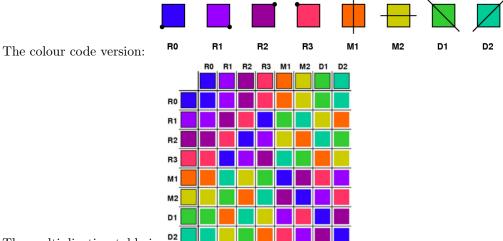
Example 2.2. Consider a square of a uniform colour. Think about a rotation of the square by 90°. After the operation, we can't even differenciate between previous and current square.

In the same way, we can easily see the square has 8 symmetries - 4 rotations, 2 mirror images and 2 diagonal flips.

Operations	Original Square	After Operation
D. — Potetion of 0° (Identity)	P W	P W
$R_0 = \text{Rotation of } 0^{\circ}(\text{Identity})$	G B	G B
D D-+-+:f 00°	P W	W B
$R_1 = \text{Rotation of } 90^{\circ}$	G B	P G
D D-4-4:f 1000	P W	B G
$R_2 = \text{Rotation of } 180^{\circ}$	G B	W P
D. Datation of 2700	P W	G P
$R_3 = \text{Rotation of } 270^{\circ}$	G B	B W
M Ventical Deflection	P W	W P
$M_1 = \text{Vertical Reflection}$	G B	B G
M Horizontal Deflection	P W	G B
$M_2 = \text{Horizontal Reflection}$	G B	P W
D — Diagonal Elip	P W	P G
$D_1 = \text{Diagonal Flip}$	G B	W B
$D_2 =$ Another Diagonal Flip	P W	B W
D ₂ – Another Diagonal Flip	G B	G P

Table 2.2. Square symmetry Group

For a bit of beauty, I should colour-code. Using that let's see the multiplication table.



The multiplication table is:

This group is called D_4 . If it is n-gon, then we call it D_n . It contains 2n elements. These are called Dihedral Groups of order 2n.

We can write a very simple sagemath code to study the group. Let's see,

```
>>> D4 = DihedralGroup(4) #with arrows mean sage code
>>> D4.is_abelian()
  0
>>> D4.order()
  8
>>> D4.list()
   [(), (1,3)(2,4), (1,4,3,2), (1,2,3,4), (2,4), (1,3), (1,4)(2,3), (1,2)(3,4)]
>>> D4("(1,3)(2,4)").order()
  2#Hence rotation by 180
>>> D4("(1,2,3,4)").order()
  4 \# rotation by 90
>>> D4.multiplication_table(names='digits')
   * 0 1 2 3 4 5 6 7
   0 0 1 2 3 4 5 6 7
     1 | 0 | 3 | 2 | 5 | 4 | 7 | 6
   2 2 6 0 4 3 7 1 5
   3 3 7 1 5 2 6 0 4
     4 5 6 7 0 1 2
   5 5 4 7 6 1 0 3 2
   6 6 2 4 0 7 3 5 1
     7 3 5
               6 2 4 0
            1
```

In[4]:= DihedralGroup[4]#this means mathematica code

 ${\tt DihedralGroup}[4]$

In[5]:= TableForm[DihedralGroup[4]//GroupMultiplicationTable,TableHeadings>Automatic]

	1	2	3	4	5	6	7	8
1	1	2	3	4	5	6	7	8
2	2	1	4	3	6	5	8	7
3	3	7	1	5	4	8	2	6
4	4	8	2	6	3	7	1	5
5	5	6	7	8	1	2	3	4
6	6	5	8	7	2	1	4	3
7	7	3	5	1	8	4	6	2
8	8	4	6	2	7	3	5	1

Let's see few useful definitions.

(Definition 2.2: Finite Groups and Order)

A group which has a finite number of elements is called a **Finite Group**. The **order** of a finite group is defined as the number of elements in the group.

All previous examples showes finite groups. Any groups with infinite elements are called **Infinite** group.

Let's see an example for an infinite group!

Example 2.3. (1D translational group T_1)

Let x represent a real variable. Here $x \in \mathbb{R}$ and it can be either a spatial coordinate or the time coordinate. For any real constant parameter a, we define an operator T(a) which acting on the coordinate x simply translates it by an amount a such that,

$$T(a)x = x + a, \quad \forall x \in \mathbb{R}$$
 (2.5)

This can be understood physically. Let's use the **active transformation**, i.e., where the point we are studying moves and not the coordinate itself.

So, we can write

$$T(a): x \quad -^{T(a)} \rightarrow \quad x' = x + a \tag{2.6}$$

We can also take T(a) as a *linear operator* satisfying eqn-2.5 with the action of T(a) leaving any constant parameter b unchanged (Remember?). This can be written as,

$$T(a)b = b (2.7)$$

Using eqn-2.5 and 2.7 we can easily prove that forms a group.

As an example,

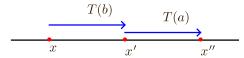
$$T(a)T(b)x = T(a)(x+b)$$

$$= T(a)x + T(a)b$$

$$= (x+a) + b$$

$$= x + a + b$$

A pictorial view is:



We can find the the differential operator representation of T(a):

$$T(a) = 1 + a\frac{d}{dx} \tag{2.8}$$

It's pretty clear, this group has infinite elements. The identity of the group is T(0) = e. Also, the identity of T(a) is given by T(-a).

We will for now not focus on this type of groups. Later, we will see them in detail.

There is a very interesting thing about finite groups.

Let's suppose g_1 is an element of some finite group. We now consider the sequence $\{g_1, g_1^2, g_1^3, \dots\}$. As, the group is finite at some point the sequence has to repeat. So, let's say $g_1^{k_1} = 0$. It's also possible $g_1^{k_2} = 0$ and so on. The **order of the element** g_1 is min (k_1, k_2, \dots) .

As an example, in Examp-2.2, the order of R_1 is 4.

Let's consider another famous type of groups. They are called **Cyclic Group**.

To understand that, let's start with the set of all integers \mathbb{Z} , with the group operation being the addition between two integers. We can easily see that it forms a group.

Now, let's consider the set $\{0, 1, 2\}$, with the group operation being: addition of two numbers modulo 3. This also forms a group. This group is written as \mathbb{Z}_3 . This is actually a set containing the remainders on division by number 3.

In a very similar way, for any integer n, we can form a set $\{0, 1, 2, 3, \dots, n-1\}$ with the operation of addition modulo n. This will always form a group. This group is called \mathbb{Z}_n (Cyclic Group of order n). Let's see the multiplication table of \mathbb{Z}_3 .

				_				
	0	1	2			e	a	
0	0	1	2		e	e	a	
1	1	2	0		a	a	b	
2	2	0	1		b	b	е	Γ

Table. With numbers Table. With symbols

Table 2.3. Muliplication table of \mathbb{Z}_3

We can recreate the same group without specifiying numbers. We can keep things abstract and just say, we have 3 elements $\{e, a, b\}$ with some binary operation \circ such that $a \circ b = e$, $a \circ a = b$ and $b \circ b = a$, along with the fact that the group is abelian. This is also \mathbb{Z}_3 but which is purely abstract.

Let's see a code for generating this multiplication tables.

Wolfram-lang plugin for GNU $T_{
m E}X_{
m MACS}$

In[4] := CyclicGroup[5]
CyclicGroup[5]
In[5] := CyclicGroup[5]//GroupGenerators
{Cycles[(1 2 3 4 5)]}

In[6] := TableForm[GroupMultiplicationTable[CyclicGroup[3]]-1, TableHeadings>{Range[0,2],Range[0,2]}]

	0	1	2
0	0	1	2
1	1	2	0
2	2	0	1

Before ending this part, let's see two more example,

Example 2.4. (Symmetry Group S_3)

Consider the group of all permutations of 3 distinguishable objects, say x, y, z. The group has 3! = 6 elements. Now, consider the element a which takes the 1st object to the 2nd object, the 2nd object to the 3rd and the 3rd to the 1st,i.e.,(a is written as $(1\ 2\ 3))$

$$a \circ (xyz) = (zxy)$$

Also, consider the element b of the group that exchanges the 1st and 2nd element, i.e., (b is written as $(1\ 2)(3)$ or just $(1\ 2)$)

$$b \circ (xyz) = (yxz)$$

Note: The operations are group elements and not the object arrangement. What will happen if we combine a and b?

The answer is:

$$ab \circ (xyz) = (zyx)$$

 $ba \circ (xyz) = (xzy)$

Here the identity will be the elements which doesn't change (xyz), i.e.,

$$e \circ (xyz) = (xyz)$$

Clearly ab \neq ba. So, S_3 is a non-abelian group.

Let's form, it's characteristic table:

$$[(), (1,3,2), (1,2,3), (2,3), (1,3), (1,2)]$$

>>> S3.multiplication_table(names=names)

*	e	UK	a	ba	a b	b
e	e	UK	a	ba	a b	b
UK	UK	e	ba	a	b	a b
a	a	a b	e	b	UK	ba
ba	ba	b	UK	a b	e	a
a b	a b	a	b	e	ba	UK
b	b	ba	a b	UK	a	e

You can rearrange it a bit more clearly and can also find (132) in terms of a and b.

Some times people use different notations also, as shown:

$$e = \begin{pmatrix} 1 & 2 & 3 \\ 1 & 2 & 3 \end{pmatrix}; a = \begin{pmatrix} 1 & 2 & 3 \\ 2 & 3 & 1 \end{pmatrix}$$

Here the first row represent your original arrangement and second one represent where each one will go. As an example, a represent $1 \rightarrow 2$, $2 \rightarrow 3$ and $3 \rightarrow 1$ (see colour code).

Example 2.5. Let's create an abstract group, i.e., without any explicit physical interpretation.

The first element is the obvious one e. Let's say the other non-trivial ones are a and b. These two are bad boys. They satisfies some conditions, those are,

$$a^3 = e ab = ba^2$$

The group is clearly non-abelian as $ba = bab^2 = b(ab)b = bba^2b = a^2b$, which implies $ab \neq ba$.

A bit of thinking let us figure out the group elements $\{e, a, a^2, b, ab, a^2b\}$ (psh! This is also symmetric Group S_3). We can also write the multiplication table (let's use sagemath for this one!):

SageMath version 10.3, Release Date: 2024-03-19

```
>>> F = FreeGroup('a, b')
>>> a,b = F.gens()
>>> G = F/[a^3,b^2, a^2*b*a^2*b]
>>> elements = G.list()
>>> elements
   (1, a, a^-1, b, a*b, a^-1*b)
>>> names = ["e","a","a^2","b","ab","a^2b"]
```

>>> G.multiplication	_table	(names=names)
----------------------	--------	---------------

*	e	a	a^2	b	ab	a^2b
e	e	a	a^2	b	ab	a^2b
a	a	e	b	a^2	a^2b	ab
a^2	a^2	a^2b	a b	a	e	b
b	b	a b	a^2b	e	a	a^2
a b	a b	b	e	a^2b	a^2	a
a^2b	a^2b	a^2	a	a b	b	e

Something we should note. Although, I am pretty sure, you guys already know, "The set of all 2×2 matrices with determinant 1 with entries from \mathbb{Q} (rational numbers), \mathbb{R} (real numbers) or even \mathbb{C} (complex numbers) forms groups. These are called Special Linear Group of 2×2 matrices over \mathbb{Q} , \mathbb{R} or \mathbb{C} respectively. (For the application part see the Appendex-A)

If you have noticed the codes, we have used something as "gen", which are generators. But what are those?,

(Definition 2.3: Generators)

A subset S of elements of a group G is said to be generate G if every element of G can be expressed as a finite product of finite powers of elements (or their inverses) of S in some order. The elements of the minimal set S that generates a group G are called the Generators of the group and S itself is called the Generating S et.

If the set S is finite then the group G is said to be finitely generated. Also, a group whose generating set contains a single element is said to be **cyclic group**. In the example-2.5, a and b are the generators.

Example 2.6. The set $\{a\}$ along with the relation $a^n = e$ (n is some positive integer) generates the cyclic group $\{e, a, a^2, \dots, a^{n-1}\}$. It's order is n. The symbol of the group is C_n .

Now, let's go further into the groups and see if there are some hidden groups inside the bigger ones. Actually even in our QFT, we will se that we have a group called "Poincare Group", but we really don't need to study the whole group. Rather, there is small part of the group called "Little Group", which is sufficient for us.

Let's try to understand what is the groups inside group.

(Definition 2.4: Subgroup)

Let H be a subset of a group G. If H is itself a group under the same binary operation as G, then H is aid to be a subgroup in G.

If a subset H of a group G is a subgroup then it is necessary that H must contain the same identity element as that of G.

What is the subgroup of S_3 ?, If you remember $S_3 = \{() = e, (1,3,2), (1,2,3), (2,3), (1,3), (1,2)\}$. I will use $a_1 = (1,2,3), a_2 = (1,3,2), a_3 = (1,2), a_4 = (2,3)$ and $a_5 = (1,3)$.

Now, let's take $H = \{e, (1, 2, 3), (1, 3, 2)\} = \{e, a_1, a_3\}$. This is indeed a subgroup (check!).

```
>>> sigma = S3("(1,2,3)")
```

>>> H = S3.subgroup([sigma])

>>> H.list()

The subgroup of S_3 is represented by Z_3 .

Another example of subgroup is the subgroup of D_4 which is $\{R_0, R_1, R_2, R_3\}$.

Theorem 2.1: Finding Subset

Let G be a group. A non-empty subset H of G is a subgroup if and only if $x, y \in H$ implies that $xy^{-1} \in H$.

Every group G always has two subgroups, the full group G and the trivial subgroup $\{1\}$ consisting of just the identity element. Any other subgroup of a group G will be called a **non-trivial proper subgroup**.

It is not always easy to find all the subgroups of a group. However, there are some subgroups which can be easily identified. For example, take any element $g \in G$. Of course g^2 will belong to G and so will any higher power of g. The inverse of g, i.e., g^{-1} , will also be in G and so will powers of g^{-1} . Thus, if we consider the set $\{\cdots, g^{-2}, g^{-1}, e, g, g^2, \cdots\}$, then it will definitely be a subgroup of G. It is called the subgroup of G generated by g and is symbolically written as $\langle g \rangle$.

Example 2.7. Consider the group \mathbb{Z} under usual addition. According to Theorem-2.1, a non-empty subset H of \mathbb{Z} is a subgroup if and only if $x - y \in H$ whenever $x, y \in H$.

(Definition 2.5: Cosets)

We can use a subgroup to divide up the elements of the group into subsets called Cosets. A right-coset of the subgroup H in the group G is a set of elements formed by the action of the elements of H on the left on a given element of G, i.e., all elements of the form Hg for some fixed g. In a smiliar manner gH represent left-coset.

Let's see an example:

Example 2.8. Let's start with the subgroup $Z_3 = \{e, a_1, a_2\}$ of the group $S_3 = \{e, a_1, a_2, a_3, a_4, a_5\}$. Remeber the operations? Let's recap:

	e	a_1	a_2	a_3	a_4	a_5
e	e	a_1	a_2	a_3	a_4	a_5
a_1	a_1	a_2	e	a_5	a_3	a_4
a_2	a_2	e	a_1	a_4	a_5	a_3
a_3	a_3	a_4	a_5	e	a_1	a_2
a_4	a_4	a_5	a_3	a_2	e	a_1
a_5	a_5	a_3	a_4	a_1	a_2	e

Table 2.4. S_3 multiplication table with the new notation.

Now, one of the right-coset of the subgroup Z_3 in the group S_3 is a_3Z_3 . This gives us:

$$a_3Z_3 = a_3\{e, a_1, a_2\} = \{a_3e, a_3a_1, a_3a_2\}$$

= $\{a_3, a_4, a_5\}$

Similarly, the left-coset of the subgroup Z_3 in the group S_3 is Z_3a_3 . This gives us:

$$Z_3a_3 = \{e, a_1, a_2\}a_3 = \{ea_3, a_1a_3, a_2a_3\}$$

= $\{a_3, a_5, a_4\}$

The number of elements in a coset is the order of H, as expected!

Note: As eH = He = H, so, H is always a coset.

From the definition of the coset, it seems that for a subgroup H, each group element g gives a different left coset gH and a different right-coset Hg. But is it not the case, as I have just shown in the example.

(Theorem 2.2: Equality of Coset)

If $g' \in gH$, i.e., g' is a member of the set gH, then g'H = gH. Similarly, if $g' \in Hg$, then Hg' = Hg. Note: This shows if the order of the group G is g. We can't have g number of cosets of type left or right.

Let's see an example:

Example 2.9. Let's foolishly forget about the previous theorem and try finding 6 cosets:

$$\begin{array}{rcl} \mathrm{eZ}_3 &=& \{e,a_1,a_2\} \\ a_1Z_3 &=& \{a_1,a_2,e\} \\ a_2Z_3 &=& \{a_2,e,a_1\} \\ a_3Z_3 &=& \{a_3,a_4,a_5\} \\ a_4Z_3 &=& \{a_4,e,a_3\} \\ a_5Z_3 &=& \{a_5,e,a_4\} \end{array}$$

You can clearly see that for the first one as $a_1 \in eZ_3$, so $a_1H = eH$ (interesting right?)

But then how do we create "Non- Overlapping" cosets! (whenever i am saying coset, remeber I am talking about non-overlapping cosets).

The process is very simple to create true cosets. The method is given below:

- i. Start with one element $g \notin H$ and form the coset gH.
- ii. Now, if H and gH don't exhaust all elements of G, we can start with other element g' that is not in either of them and form g'H.
- iii. Continue this process until you exhaust all elements of G.

As an examle, start with $a_3 \notin Z_3$. This gives us the coset $\{a_3, a_4, a_5\}$. See $Z_3 \cup a_3 Z_3 = G$ and $Z_3 \cap a_3 Z_3 = \emptyset$. So, only 2 subsets are there.

Every element of G must belong to one and only one coset (only consider one type of coset). Let's use sage to see the example once again:

```
>>> S3.list()
   [(), (1,3,2), (1,2,3), (2,3), (1,3), (1,2)]
>>> sigma = S3("(1,2,3)")
>>> Z_3_sub = S3.subgroup([sigma]); Z_3_sub.list()
   [(), (1,2,3), (1,3,2)]
>>> S3.cosets(Z_3_sub,'right')
   [[(), (1,2,3), (1,3,2)], [(2,3), (1,3), (1,2)]]
   See onlt two cosets are there as we have found!
```

The previous discussion tells us, for finite groups, the order of a subgroup H must be a factor of order of G.

It is also sometimes useful to think about the coset-space, G/H defined by regarding each coset as a single element of the space, i,.e.,

$$G/H = \{gH: g \in G\}$$

similarly $H \setminus G = \{ \text{Hg: } g \in G \}.$

For our example: $S_3/Z_3 = \{Z_3, a_3Z_3\} = \{\{e, a_1, a_2\}, \{a_3, a_4, a_5\}\}.$

(Definition 2.6: Invariant or Normal Subgroup

A subgroup H of G is called an invarinat or normal subgroup if for **every** $g \in G$, gH = Hg

This means for every $g \in G$ and $h_1 \in H$, there exist an $h_2 \in H$ such that $h_1g = gh_2$ or $gh_2g^{-1} = h_1$. The trivial subgroups e and G are invariant for any group. This is true for Z_3 also as,

$$\begin{array}{lll} \mathrm{eZ}_3 &=& \{e,a_1,a_2\} &=& \{e,a_1,a_2\} \\ a_1Z_3 &=& \{a_1,a_2,e\} &=& \{a_1,a_2,e\} \\ a_2Z_3 &=& \{a_2,e,a_1\} &=& \{a_2,e,a_1\} \\ a_3Z_3 &=& \{a_3,a_4,a_5\} &=& \{a_3,a_4,a_5\} \\ a_4Z_3 &=& \{a_4,e,a_3\} &=& \{a_4,e,a_3\} \\ a_5Z_3 &=& \{a_5,e,a_4\} &=& \{a_5,e,a_4\} \end{array}$$

However, set $\{e, a_4\}$ is a subgroup of G which is not invariant. The reason is $a_5\{e, a_4\} = \{a_5, a_1\}$ but $\{e, a_4\}a_5 = \{a_5, a_2\}$.

If H is invariant, tehn we can regard the coset space as a group. The operation(multiplication) law in G gives the natural law on the cosets, Hg:

$$(Hg_1)(Hg_2) = (Hg_1Hg_1^{-1})(g_1g_2)$$
 (2.9)

But is H is invariant $Hg_1Hg_1^{-1} = H$, so the product of elements in two cosets is in the coset represented by the product of the elements. In this case, the **coset space**, G/H, is called the **factor group** of G by H.

What is the factor group S_3/Z_3 ?, the answer is $Z_2 = \{e, a_3\}$.

The **center of a group** G is the set of all elements of G that commute with all elements of G. The center is always an abelian, invariant subgroup of G. However, it may be trivial, consisting only of the identity, or of the whole group.

There is one other concept, related to the idea of an invariant subgroup, that will be useful. Notice that the condition for a subgroup to be invariant can be written as,

$$gHg^{-1} = H; \forall g \in G \tag{2.10}$$

```
>>> S3.list()
   [(), (1,3,2), (1,2,3), (2,3), (1,3), (1,2)]
>>> Z3_sub = S3.subgroup([S3("()"), S3("(1,3,2)"),S3("(1,2,3)")]); Z3_sub.list()
   [(), (1,3,2), (1,2,3)]
>>> print(Z3_sub.is_normal())
   True
>>> Z_ano_sub = S3.subgroup([S3("()"), S3("(2,3)")]); Z_ano_sub.list()
   [(), (2,3)]
>>> print(Z_ano_sub.is_normal())
   False
>>> S3.center().list()
   [()]
```

Elements of any group can be divided into disjoint subsets through a property called Conju-gation. An element x of a group is said to be conjugate to an element y if there exists a group element g which satisfies,

$$x = gyg^{-1}$$

The existence of such an element g will be represented by $x \sim y$ (x is conjugate to y). We can think it as a sort of equivalence. It has some following properties:

- i. Any element x is conjugate to iself, i.e., $x \sim x$.
- ii. If $x \sim y$ then $y \sim x$.
- iii. If $x \sim y$ and $y \sim z$, then $x \sim z$.

As we know, Any equivalence relation in a set divides the set into disjoint subsets, where each subset contains elements which are related.

As groups are also sets with just additional properties, in the context of groups, the elements of any subset will be conjugate to one another. These subsets are called **Conjugacy Classes**.

So, If we consider sets rather than subgroups satisfying same condition,

$$gSg^{-1} = S, \forall g \in G \tag{2.11}$$

Such sets are called **Conjugacy Classes**.

Note: No element can belong to more than one class, so in this sense the classes are disjoint. A subgroup that is a union of conjugacy classes is invariant.

Example 2.10. For S_3 , let's see some for some subsets,

$$S = \{e\} \implies \text{gSg}^{-1} = S = \{e\}$$

$$S = \{a_1, a_2\} \implies \text{gSg}^{-1} = S = \{a_1, a_2\}$$

$$S = \{a_3, a_4, a_5\} \implies \text{gSg}^{-1} = S = \{a_3, a_4, a_5\}$$

Note 2.1. The is a very deeper meaning of Normal Subgroup and Equivalent Classes / Conjugacy Classes. Let's try to understand that.

Let's suppose, H is a normal subgroup of G, then it means gH and Hg sets are same for any $g \in G$. This also means,

$$H = qHq^{-1}$$

We also know H and gHg^{-1} are conjugate subgroups. But here they are exactly equal if H is invarinat subgroup. This means H contains all conjugates of any of its elements.

A normal subgroup therefore contains whole equivalence classes. If someone wants to search for normal subgroups, the steps would be to identify the classes first and then make unions of such classes and check whether the subset thus formed is a group by itself.

2.1.2 Homomorphism and Representations

In the previous discussion, we have seen \mathbb{Z}_3 can be described by a complete abstract notation. But it helps us if we use numbers. Also, if you rearrange multiplication table of S_3 or the table of the example-2.5, you will see one is resembling other.

Here multiplication table is the key. We can say, there exists a one-to-one correspondence between the elements of S_3 and that of the other group. Such kind of correspondence is called a homomorphism between two groups.

```
(Definition 2.7: Homomorphism)
```

If two groups G and G' are related by a map $\phi: G \to G'$ such that $g_1g_2 = g_3$ in G implies $\phi(g_!)\phi(g_2) = \phi(g_3)$ in G', then ϕ is said to be a homomorphism from G to G'.

As, an example, commsider \mathbb{Z} , the group of integers under addition and \mathbb{Q}^* , the group of non-zero rational numbers under multiplication. The mapping $\phi \colon \mathbb{Z} \to \mathbb{Q}^*$ given by $\phi(x) = 2^x$ is a homomorphism as $\phi(x+y) = 2^{x+y} = 2^x 2^y = \phi(x)\phi(y)$.

For our previous example of S_3 and the other group, we can find a homomorphism using sage also.

Let's see a theorem which is very useful:

(Theorem 2.3: Some Theorems)

Let $\phi: G \to H$ be a group homomorphism. Then,

- 1. $\phi(e_q) = e_{q'}$, i.e., the identity of G is mapped to the identity of G'.
- 2. $\phi(x^{-1}) = \phi(x)^{-1}$ for $x \in G$.
- 3. If $\phi: G \to G'$ and $\psi: G' \to G''$ are group homomorphisms then the composite map $\psi \circ \phi: G \to G''$ is also a homomorphism.

So, homomorphism is sort of mapping.

Let's see one more example.

Example 2.11. Let $C_2 = \{e_{C2}, A\}$ where C_2 is the cyclic group of order 2 in our notation and e_{C2} is the identity of C_2 . Consider a function ϕ from group in example-2.5 to C_2 defined as,

$$\phi\left(e\right) = \phi\left(a\right) = \phi\left(a^{2}\right) = e_{C2}$$

$$\phi(b) = \phi(ba) = \phi(ba^2) = A$$

Then, ϕ is a homomorphsim.

Note that, while defining homomorphism through a map from one group to another, we did not assume anything regarding whether the map is injective, surjective or bijective.

$ig({ m Definition} \,\, 2.8 { m :} \,\, { m Isomorphism} ig)$

If the map happens to be bijective, i.e., one-to-one and onto , i.e., If a homomorphism ϕ : $G \to G'$ is invertible, then it is called an **Isomorphism**.

The groups G and G' are said to be isomorphic to each other.

So, according to the definition, there exists an isomorphism between two groups, the elements of each group is in one-to-one correspondence with the other.

There is therefore no perceptible difference between the two groups, and we can call the two groups to be the same group.

The map involved in a homomorphism need not be bijective. However, any homomorphism from G to G' defines two important subgroups- one of G and one of G'. The subgroup of G' defined by a homomorphism is the image group, i.e., the image of the map in G', i.e.,

$$\phi(G) = \{ y \in G' | y = \phi(a) \text{ for some } a \in G \}$$

$$(2.12)$$

It is easy to prove that it is a subgroup of G'. If $\phi(G) = G'$, then the map is surjective.

The subgroup of G that is important in this context is called the **Kernal** of the map. It is defined as,

$$\ker(\phi) = \{ a \in G \mid \phi(a) = \phi(e) \} \tag{2.13}$$

So, basically **Kernal** is the list of all elements of **G** which maps onto the identity of **G**'. Remember eqn-2.11, similar to that, the mapping

$$G \to qGq^{-1} \tag{2.14}$$

for a fixed g is also interesting. It is called an *Inner Automorphsim*. An *Automorphism* is a one-to-one mapping of a group onto itself that preserves the binary law. If in the last equation $g \notin G$, then it is called *Outer Automorphism*.

2.1.3 Representation

Upto this we have talked about groups in-terms of abstract ideas or some physical notion like rotation. As an example, thing about the group D_4 . We have talked in terms of rotation, reflection and all. We are absolutly fine and can do all things by just looking into the multiplication table.

But is there a way to not always look into the table? Someway here it will be easier for us to do the calculations easily?,

There is:

Let's start remembering a very interesting fact! "Our vector space are actually groups". So, if we can map our known groups into these vector spaces, our calculations will be much more simpler!

As, an example, let's see the group of the symmetry of square, i.e., D_4 . Using the idea of matrices, we know how to represent rotations, reflections in terms of matrices.

Group Action	Matrice Representation
Rotation by $0^{\circ}(R_0)$	$\left(\begin{array}{cc} 1 & 0 \\ 0 & 1 \end{array}\right)$
Rotation by $90^{\circ}(R_1)$	$\left(egin{array}{cc} 0 & 1 \\ -1 & 0 \end{array} ight)$
Rotation by $180^{\circ}(R_2)$	$\left(egin{array}{cc} -1 & 0 \ 0 & -1 \end{array} ight)$
Rotation by $270^{\circ}(R_3)$	$\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$
Vertical Reflection (M_1)	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$
Horizontal Reflection (M_2)	$\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$
Diagonal Flip (D_1)	$\left(egin{array}{cc} 0 & -1 \ -1 & 0 \end{array} ight)$
Another Diagonal $Flip(D_2)$	$\left(\begin{array}{cc} 0 & 1 \\ 1 & 0 \end{array}\right)$

Let's see if it works fine. Looking into the multiplication table, we know $R_1R_2 = R_3$.

Try doing the matrix multiplication. You will se it gives the correct equality. This will hold for all the elements!

So, if we remember the matrices (which can be easily done, watch 3b1b linear algebra playlist), we don't need to know the multiplication table at all.

Due to this reason and many more as we will see later, we always want to find this sort of representation for abstract groups in terms of matrices or easy to handle functions. In very vague term these is what is called "Representation".

-(Definition 2.9: Representation)

A Representation of G is a mapping, D of the elements of G onto a set of linear operators with the following properties:

- 1. D(e) = 1, where 1 is the identity operator in the space on which the linear operator act.
- 2. $D(g_1)D(g_2) = D(g_1g_2)$, in other words the group multiplication law is mapped onto the multiplication (matrix multiplication) in the linear space on which the linear operators act.

We can also define this in more mathematical sense using Aut(V). Note that it denotes the space of automorphisms on V, which are maps from V to itself. As long as we are dealing with finite groups, we will only consider linear automorphisms.

"A representation of a group G is a homomorphism $\Gamma: G \to \operatorname{Aut}(V)$, where V is a linear space of dimension n, is called a representation of G". A representation is said to be faithful if it is one-one, i.e., no two distinct elements map to the same matrix. The dimension of the space V corresponding to the representation is called the **degree** of the representation.

Let's see all the group representations which we have discussed upto this point

Example 2.12. For \mathbb{Z}_3 , we can take D(e or 0) = 1, $D(a \text{ or } 1) = e^{2\pi i/3}$ and $D(b \text{ or } 2) = e^{4\pi i/3}$. The dimension of this representation is 1.

We can also find a matrix representation,

$$D(e) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} D(a) = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} D(b) = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$$

This representation was constructed directly from the multiplication table by the following trick. Take the group elements themselves to form an orthogonal basis for a vector space $|e\rangle$, $|a\rangle$ and $|b\rangle$. Now define,

$$D(g_1)|g_2\rangle = |g_1g_2\rangle \tag{2.15}$$

Try showing that this is a representation. It is called *regular representation*. See the classnote for more detail on the creation of the matrices or see example-2.13 for detailed method.

Evidently, the dimension of the regular representation is the order of the group.

The matrices written are then constructed as follows:

$$|e_1\rangle \equiv |e\rangle \quad |e_2\rangle \equiv |a\rangle \quad |e_3\rangle \equiv |b\rangle$$
 (2.16)

$$[D(g)]_{ij} = \langle e_i | D(g) | e_j \rangle \tag{2.17}$$

The matrices are the matrix elements of the linear operators. The last equation is very simple but very general.

This works for any representation, not just the regular representation.

The basic idea is just the insertion of a complete set of intermediate states. The matrix corresponding to a product of operators is the matrix product of the matrices corresponding to the operators

$$[D(g_{1}g_{2})]_{ij} = [D(g_{1})D(g_{2})]_{ij}$$

$$= \langle e_{i}|D(g_{1})D(g_{2})|e_{j}\rangle$$

$$= \sum_{r} \langle e_{i}|D(g_{1})|e_{r}\rangle\langle e_{r}|D(g_{2})|e_{j}\rangle$$

$$= \sum_{r} [D(g_{1})]_{ir}[D(g_{2})]_{rj}$$
(2.18)

For detailed method of finding the matrice form, see the classnote or example below.

Example 2.13. Let's start with S_3 group. The elements are e, $a_1 = (1, 2, 3), a_2 = (3, 2, 1), a_3 = (1, 2), a_4 = (2, 3)$ and $a_5 = (3, 1)$.

Start by forming the regular representation. For this we will use our method. Choose, 6, unit vectors.

$$|e\rangle = \begin{pmatrix} 1\\0\\0\\0\\0\\0 \end{pmatrix} \qquad |a_1\rangle = \begin{pmatrix} 0\\1\\0\\0\\0\\0 \end{pmatrix} \qquad |a_2\rangle = \begin{pmatrix} 0\\0\\1\\0\\0\\0\\0 \end{pmatrix}$$

$$|a_3\rangle = \begin{pmatrix} 0\\0\\0\\0\\1\\0\\0 \end{pmatrix} \qquad |a_4\rangle = \begin{pmatrix} 0\\0\\0\\0\\0\\1\\0 \end{pmatrix} \qquad |a_5\rangle = \begin{pmatrix} 0\\0\\0\\0\\0\\0\\1\\0 \end{pmatrix}$$

Now, we see the multiplication table,

	e	a_1	a_2	a_3	a_4	a_5
e	e	a_1	a_2	a_3	a_4	a_5
a_1	a_1	a_2	e	a_5	a_3	a_4
a_2	a_2	е	a_1	a_4	a_5	a_3
a_3	a_3	a_4	a_5	e	a_1	a_2
a_4	a_4	a_5	a_3	a_2	e	a_1
a_5	a_5	a_3	a_4	a_1	a_2	e

Using this table and $D(g_1)|g_2\rangle = |g_1g_2\rangle$, we have:

$$D(a_1)|a_2\rangle = |a_1a_2\rangle = |e\rangle$$

$$D(a_1)|a_1\rangle = |a_1a_1\rangle = |a_2\rangle$$

$$D(a_1)|a_3\rangle = |a_1a_3\rangle = |a_5\rangle$$

$$D(a_1)|a_4\rangle = |a_1a_4\rangle = |a_3\rangle$$

$$D(a_1)|a_5\rangle = |a_1a_5\rangle = |a_4\rangle$$

$$D(a_1)|e\rangle = |a_1e\rangle = |a_1\rangle$$

Using this, we get,

$$D(a_1) = \begin{pmatrix} 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix}$$
(columnwise)
$$\begin{bmatrix} -a_1 - a_2 - e - a_5 - a_3 - a_4 \end{bmatrix}$$

Similarly, we can do the same for others,

Using this, we get,

This is the regular representation. Now, just diagonalize these and we are done. SageMath version 10.3, Release Date: 2024-03-19

```
>>> S3 = SymmetricGroup(3)
>>> def regular_representation(G):
        elements = G.list();n = len(elements)
        element_to_index = {elements[i]: i for i in range(n)}
        representation = []
        for g in G:
            M = matrix(QQ, n)
            for i in range(n):
                h = elements[i];g_h = g * h
                M[i, element_to_index[g_h]] = 1
            representation.append(M)
        return representation
    regular_rep_S3 = regular_representation(S3)
    for i, matrix in enumerate(regular_rep_S3):
        print(f"Matrix for element {S3.list()[i]}:\n{matrix}\n")
  Matrix for element ():
   [1 0 0 0 0 0]
   [0 1 0 0 0 0]
   [0 0 1 0 0 0]
   [0 0 0 1 0 0]
   [0 0 0 0 1 0]
   [0 0 0 0 0 1]
  Matrix for element (1,3,2):
   [0 1 0 0 0 0]
   [0 0 1 0 0 0]
   [1 0 0 0 0 0]
   [0 0 0 0 0 1]
   [0 0 0 1 0 0]
   [0 0 0 0 1 0]
```

```
Matrix for element (1,2,3):
[0 0 1 0 0 0]
[1 0 0 0 0 0]
[0 1 0 0 0 0]
[0 0 0 0 1 0]
[0 0 0 0 0 1]
[0 0 0 1 0 0]
Matrix for element (2,3):
[0 0 0 1 0 0]
[0 0 0 0 1 0]
[0 0 0 0 0 1]
[1 0 0 0 0 0]
[0 1 0 0 0 0]
[0 0 1 0 0 0]
Matrix for element (1,3):
[0 0 0 0 1 0]
[0 0 0 0 0 1]
[0 0 0 1 0 0]
[0 0 1 0 0 0]
[1 0 0 0 0 0]
[0 1 0 0 0 0]
Matrix for element (1,2):
[0 0 0 0 0 1]
[0 0 0 1 0 0]
[0 0 0 0 1 0]
[0 1 0 0 0 0]
[0 0 1 0 0 0]
[1 0 0 0 0 0]
See, these are matching!.
```

Example 2.14. Let's consider another group with two elements e and a, with the following multiplication table,

 e
 a

 e
 e

 a
 a

Table 2.5. Interchange group

We can assign 2×2 matrix corresponding to each group element as follows,

$$e \rightarrow D(e) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$
 , $a \rightarrow D(a) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ (2.19)

Using these matrices, you can verify the multiplication table.

Let's see this in more detail.

A matrix operates on vectors in a vector space. For the example above, each of these vectors will be a column matrix with 2 elements, i.e., an object of form

$$\psi = \begin{pmatrix} p \\ q \end{pmatrix} \tag{2.20}$$

Such objects on which the group elements operate will be called states in our discussion. As we know group elements are symmetry operators. They are helpful in describing symmetries. And the states somehow characterize the system on which we perform symmetry operations.

The operation of the two matrices defined above produces the following effects on a typical column matrix:

$$D(e)\psi = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} p \\ q \end{pmatrix} = \begin{pmatrix} p \\ q \end{pmatrix}$$

$$D(a)\psi = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} p \\ q \end{pmatrix} = \begin{pmatrix} q \\ p \end{pmatrix}$$
(2.21)

So, the action of the element a interchanges the 2 elements of ψ , whereas the action of e doesn't have any effect.

Note 2.2. The components of a vector depend on the basis chosen in a vector space. Let us change the basis in the 2-D vector space that we have been using. Let's use an unitary matrix to change the basis.

$$U = \frac{1}{\sqrt{2}} \left(\begin{array}{cc} 1 & 1 \\ 1 & -1 \end{array} \right)$$

Then, in the new basis, the state ψ will take the form,

$$\psi' = U\psi = \frac{1}{\sqrt{2}} \begin{pmatrix} p+q \\ p-q \end{pmatrix} \equiv \begin{pmatrix} p' \\ q' \end{pmatrix}$$

The representation matrices for the group element will also be affected. The forms will be,

$$D'(e) = \mathrm{UD}(e)U^{\dagger} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$
$$D'(a) = \mathrm{UD}(a)U^{\dagger} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Here remember $U^{\dagger}U = 1$

2.1.3.1 Reducibility

Consider now an arbitrary representation of an arbitrary group G, in which D(g) is the matrix that the group element g is mapped to. These matrices act on states, which can be written as column vectors in the vector space. A state ψ , under the action of the matrix D(g), will give a state ψ' that is also a member of the **same vector space**.

Now, to go further, let's discuss what do we mean by Vector Subspace.

(Definition 2.10: subspace)

Let's suppose we have a vector space V over the field F and set S, i.e., $V = (S, F, +, \dot{})$. If we can define a subset of set S, and it satisfies all the condition of vectors over field F, then the subset is called Subspace of the vector space V.

Any vector space has at least 2 subspace. They are $\{0\}$ and the whole space. These are called trivial subspaces.

Example 2.15. Think about points in the 3-D space \mathbb{R}^3 constitue a real vector space. If we take a 2-D plane in this space passing through the origin, that is an \mathbb{R}^2 SUBSPACE of \mathbb{R}^3 .

- (Definition 2.11: Invariant Subspace)

Let $T: V \to V$ be a linear map. A subspace W of V is said to be invariant under T if T maps W into itself, i.e., $w \in W \Rightarrow T(w) \in W$.

Let's see an example,

Example 2.16. Let's see a 3D space. We define a map $T(x, y, z) = (x\cos(\theta) - y\sin(\theta), x\sin(\theta) + y\cos(\theta), z)$. This rotate any point w.r.t z – axis by angle θ .

Now, any point on 2D x-y plane, remains on x-y plane. So, x-y plane is the invariant subspace under T.

Definition 2.12: Projection/Projection Operator

Let P be a linear operator on V from V to V, i.e, $P: V \to V$ for which $P^2 = P$. Then P is a projection operator or projection.

Let U and W are subspaces of V along with projection operator P such that U = P(V).

We say V is said to be the direct sum of U and W, i.e., $V = U \oplus W$ if and only if,

i.
$$V = U + W$$

ii.
$$U \cap W = \{0\}$$

Proof. Let U = Im(P) and W = ker(P). Also, suppose $v \in V$, then P(v) = u

w = v - P(v), which gives v = w + P(v) = w + u.

Also,
$$P(w) = P(v - P(v)) = P(v) - P^{2}(v) = 0$$
,

Then, v = u + w, hence, V = U + W.

let now, $k \in U \cap W$, then P(k) = k and P(k) = 0 as $k \in U \& k \in W$

Hence,
$$k = P(k) = 0 \Rightarrow U \cap W = \{0\}$$

This can also be written as, if there exist subspaces U_1 and U_2 of V such that every element of v in V can be uniquely expressed as the sum $u_1 + u_2$ where $u_i \in U_i$, then V is said to be **direct** sum of the subspaces U_1 and U_2 , i.e.,

$$V = U_1 \oplus U_2 \tag{2.22}$$

Using this ideas, suppose we divide the elements of the state ψ into two parts, and write the effect of D(g) in this way,

$$\begin{pmatrix} \psi_1' \\ \psi_2' \end{pmatrix} = \begin{pmatrix} D_1(g) & D_2(g) \\ D_3(g) & D_4(g) \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}$$
 (2.23)

 ψ_1 or ψ_2 are not single numbers. They can be column matrices each having at least 1 element (same is true for dashed ones). Similarly, $D_i(g)$'s are also block matrices with appropriate numbers of rows and columns so that the matrix multiplication on the right side is valid.

We are basically breaking V into two subspaces V_1 and V_2 with $\psi_1 \in V_1$ and $\psi_2 \in V_2$.

As we know to be a representation, we should have,

$$\begin{pmatrix} D_1(g_i) & D_2(g_i) \\ D_3(g_i) & D_4(g_i) \end{pmatrix} \begin{pmatrix} D_1(g_j) & D_2(g_j) \\ D_3(g_j) & D_4(g_j) \end{pmatrix} = \begin{pmatrix} D_1(g_ig_j) & D_2(g_ig_j) \\ D_3(g_ig_j) & D_4(g_ig_j) \end{pmatrix}$$
(2.24)

or

$$D_1(g_ig_j) = D_1(g_i)D_1(g_j) + D_2(g_i)D_3(g_j)$$
 (2.25)

$$D_2(g_ig_j) = D_1(g_i)D_2(g_j) + D_2(g_i)D_4(g_j)$$
 (2.26)

$$D_3(g_ig_i) = D_3(g_i)D_1(g_i) + D_4(g_i)D_3(g_i)$$
 (2.27)

$$D_4(g_ig_i) = D_3(g_i)D_2(g_i) + D_4(g_i)D_4(g_i)$$
 (2.28)

Suppose, V_1 is the *invariant subspace*. Then it implies if $\psi_2=0$ then from eqn-2.23, then $\psi_2'=0$ as well. From the eqn-2.23, this will happen if,

$$D_3(g_i) = 0 \,\forall i \tag{2.29}$$

This actually has pretty huge significance. From eqn-2.25, we can see,

$$D_1(g_i)D_1(g_j) = D_1(g_ig_j) \,\forall i,j \tag{2.30}$$

It shows that if we take any state from the subspace V_1 , i.e., states in V with the restriction $\psi_2=0$, then for these states the matrices $D_1(g)$ themselves form a representation of the group elements on the vector space V_1 , with

$$\psi_1' = D_1(q)\psi_1 \tag{2.31}$$

The map to the vector space V is called a **Reducible Representation** of the group G, in the sense that V contains a non-trivial subspace in which a representation can also be defined. Any representation that cannot be reduced in this manner is called an **Irreducible Representation**. A visual picture for the matrix will look like,



Figure 2.1. Schematic form of matrices that yield a reducible space. Left shows reducible repsn and right shows completely reducible.

Normally left fig-2.1, is what reducible representation looks like. A representation will also be called reducible if we can change the basis such that ψ becomes $S\psi$ and the matrices $D(g_i)$ becomes $SD(g_1)S^{-1}$ and it looks like the left figure.

-(Definition 2.13: Completely Reducible)

A matrix representation $D(g_i)$ of a group is called Completely Reducible if the matrix for all g_i looks like Fig-2.1 (right side), i.e., have the form, (for $\forall i$)

$$D_2(g_i) = 0$$
 and $D_3(g_i) = 0$ (2.32)

or there exists a matrix S such that all matrices $SD(g_i)S^{-1}$ have the specified form.

Note 2.3. As already mentioned the idea of group representation are so powerful as they live in linear vector space. The wonderful thing about linear space is that we are free to choose to represent the state in a more conventional way by making a linear transformation. As long as the transformation is *invertible*, the new states are as good as the old ones. These are called Similarity Transformation.

So, to create a new representation from old one, we use,

$$D(g) \rightarrow D'(g) = SD(g)S^{-1}$$

or $D'(g) = S^{-1}D(g)S$

D(g) and D'(g) are called equivalent representations.

So, once again let's it be very clear: A represention is reducible if it has an invariant subspace, which means that the action of $D(g_i) \forall i$ on any vector in the subspace is still in the subspace (as discussed above).

This can be written in terms of projection operator P onto the subspace:

$$D(g_i)P = P \quad \forall g_i \in G \tag{2.33}$$

As discussed, representation is completely reducible if it is equivalent to a representation whose matrix elements have the form,

$$\begin{pmatrix}
D_1(g) & 0 & \dots \\
0 & D_2(g) & \dots \\
\vdots & \vdots & \ddots
\end{pmatrix}$$
(2.34)

where $D_i(g)$ is irreducible $\forall i$. This is block diagonal form as shown in Fig- 2.1(right-side).

This can only be done if there is invariant subspace. A representation in **block diagonal form** is said to be the direct sum of the subrepresentation, $D_i(g)$,

$$D_1 \oplus D_2 \oplus \cdots \tag{2.35}$$

In transforming a representation to block diagonal form, we are decomposing the original representation into direct sum of it's irreducible components. So, we can rephrase the completely reducible representation is: A completely reducible representation can be decomposed into a direct sum of irreducible representations. Again, it should be very clear that, if a representation is completely reducible, then each subspace should have one projection operator corresponding to it.

Example 2.17. Let's start with an example.

Suppose, we take our simple group $\mathbb{Z}_3 = \{e, a, b\}$ with $a^2 = b$ and $b^2 = a$. As we can easily see from the previous example-2.12,

$$D(e) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} D(a) = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} D(b) = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$$

The regular representation of \mathbb{Z}_3 has an invariant subspace project by,

$$P = \frac{1}{3} \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix} \tag{2.36}$$

This can be easily checked:

 $\label{eq:wolfram-lang} \begin{array}{lll} \text{Wolfram-lang plugin for GNU $T_E\!X_{MACS}$} \\ \text{In[11]:= De = $\{1,0,0\},\{0,1,0\},\{0,0,1\}\};$} \\ \text{Da = $\{0,0,1\},\{1,0,0\},\{0,1,0\}\};$} \\ \text{Db = $\{0,1,0\},\{0,0,1\},\{1,0,0\}\};$} \\ \text{In[16]:= P = $(1/3)*{\{1,1,1\},\{1,1,1\},\{1,1,1\}\};$}} \end{array}$

In [20] := Da.P
$$\begin{pmatrix} \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{pmatrix}$$

In[10] := P
$$\begin{pmatrix} \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{pmatrix}$$

So, as $D(g)P = P \forall g \in G$. The restriction of the representation to the invariant subspace is itself a representation.

In this example, the representation is not in completely reducible form. Let's do that , we use S matrix for the conversion,

$$S = \frac{1}{3} \begin{pmatrix} 1 & 1 & 1 \\ 1 & w^2 & w \\ 1 & w & w^2 \end{pmatrix}$$
 with $w = \exp(2\pi i/3)$

Then,

In[21]:= w = Exp[2*Pi*I/3]
$$e^{\frac{2i\pi}{3}}$$
In[60]:= S = {{1,1,1},{1,w^2,w},{1,w,w^2}}/3
Sinv = Inverse[S]
$$\left(\frac{1}{3} \quad \frac{1}{3} \quad \frac{1}{3} \quad \frac{1}{3} \quad \frac{1}{3} \quad \frac{1}{3}e^{\frac{2i\pi}{3}} \quad \frac{1}{3}e^{\frac{2i\pi}{3}} \quad \frac{1}{3}e^{\frac{2i\pi}{3}} \quad \frac{1}{3}e^{-\frac{2i\pi}{3}} \quad \frac{1}{3}e^{-\frac{2i\pi}{3}}$$

$$\text{Out [64]} = \begin{pmatrix} 1 & 1 & 1 \\ 1 & \frac{-\frac{1}{9} + \frac{1}{9}e^{-\frac{2i\pi}{3}}}{\frac{1}{9}e^{\frac{2i\pi}{3}} - \frac{1}{9}e^{-\frac{2i\pi}{3}}} & \frac{\frac{1}{9} - \frac{1}{9}e^{\frac{2i\pi}{3}}}{\frac{1}{9}e^{\frac{2i\pi}{3}} - \frac{1}{9}e^{-\frac{2i\pi}{3}}} \\ 1 & \frac{\frac{1}{9} - \frac{1}{9}e^{\frac{2i\pi}{3}}}{\frac{1}{9}e^{\frac{2i\pi}{3}} - \frac{1}{9}e^{-\frac{2i\pi}{3}}} & \frac{-\frac{1}{9} + \frac{1}{9}e^{-\frac{2i\pi}{3}}}{\frac{1}{9}e^{\frac{2i\pi}{3}} - \frac{1}{9}e^{-\frac{2i\pi}{3}}} \end{pmatrix}$$

In[70]:= Danew = Simplify[S.Da.Sinv]

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & \frac{\sqrt{3}+i}{-\sqrt{3}+i} & 0 \\ 0 & 0 & -\frac{1}{1+(-1)^{2/3}} \end{pmatrix}$$

In[66]:= Dbnew = Simplify[S.Db.Sinv]

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & -\frac{1}{1+(-1)^{2/3}} & 0 \\ 0 & 0 & \frac{\sqrt{3}+i}{-\sqrt{3}+i} \end{pmatrix}$$

In[67]:= Denew=Simplify[S.De.Sinv]

$$\left(\begin{array}{ccc}
1 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & 1
\end{array}\right)$$

This gives,

$$D'(e) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} D'(a) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & w & 0 \\ 0 & 0 & w^2 \end{pmatrix} D'(b) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & w^2 & 0 \\ 0 & 0 & w \end{pmatrix}$$

See, we get the block diagonal form.

What does these things stands for?

Well, let's take the a_{11} elements of each matrices.

$$D_1(e) = 1$$

 $D_1(a) = 1$
 $D_1(b) = 1$

This is the trivial representation.

Take a_{22} elements,

$$D_2(e) = 1$$

$$D_2(a) = w$$

$$D_2(b) = w^2$$

Using this if we make a cayley table,

	e=1	a = w	$b = w^2$
e=1	e	w	w^2
a = w	w	w^2	1
$b = w^2$	w^2	1	w

This is exactly the cayley table of \mathbb{Z}_3 , means each "block" or "diagonal" represent a representation of the \mathbb{Z}_3 group.

Crazy Right?!

Same will happen if we take the last block or element.

Let's see few more example:

Example 2.18. (Group of Integers under Addition)

Let's say, we have two elements $x, y \in I$, and $x \circ y = xy = x + y$. This group is infinite and so we can't really create a multiplication table. But it really doesn't matter as everything is specified by the above rule.

Now, consider a representation of the group,

$$D(x) = \left(\begin{array}{cc} 1 & x \\ 0 & 1 \end{array}\right)$$

Is this a reducible representation?, The answer is yes!

To see this, take the projection matrix P (we will learn later how to find these):

$$P = \left(\begin{array}{cc} 1 & 0 \\ 0 & 0 \end{array}\right)$$

We can clearly see, D(x)P = P, hence, our representation is reducible. But is it completely reducible?, To find the answer, let's first see the diagram below:

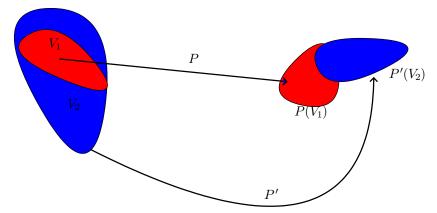


Figure 2.2. Projection of two subspaces

See, let's say D(x) is the representation corresponding to V space. Now, as the condition D(x)P = P holds, we can say, a subspace V_1 of V (corresponding to P), is an invariant subspace. But what about the other part?

As we know the projection operator for the other part is $\mathbb{I} - P$ (Think this as quantum mechanical operator, then it will be clear).

So, take,

$$P' = \mathbb{I} - P = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

It can be easily seen, $D(x)P' \neq P'$, hence, the subspace corresponding to $P' = \mathbb{I} - P$ is not an invariant subspace. Hence, D(g) is **not completely reducible**. Hence, It has the form of Fig-2.1 left side and not of right side.

Appendix A

Molecular Symmetry

To see the beautiful applications of Group Theory in different aspects of physics and also due to some requests from some students, I am adding this part.

Here we will see symmetries possessed by molecules. Here by symmetry we are talking about the **translations**, **reflections** and **rotations**^{A.1}.

Let's try to see these things.

A.1 Molecular Symmetries

Any rigid body with symmetry can be transformed to itself by doing nothing, i.e., e (Identity). It must be in the group so let's just start with this one.

What could be the other transformations? For this remember our square example. We had few rotation operations (R_1, R_2, R_3) . For molecules also it's true.

Let's see an example to define these:

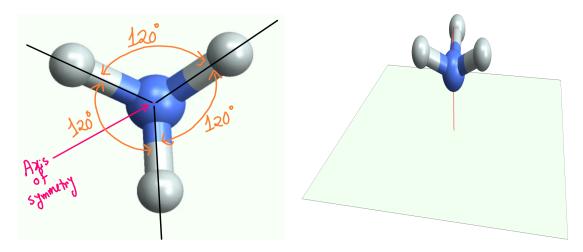


Figure A.1. Ammonia Molecule

Look into the picture above of Ammonia Molecule. See the picture in the right side, there is a molecule and a axis (red one). In the left side, there is the same image but from the top view.

Notice something?, there is a beautiful symmetry w.r.t the red axis. Any rotation of $120^{\circ} = \frac{2\pi}{3}$ wr.t to the axis seems keeps things same (visually), i.e., symmetry! This happens for 2 rotations and 3^{rd} one brings back the molecule on it's initial state, i.e., identity.

—(Definition A.1: n-Fold Axis)

A molecular having an axis of symmetry about which, if the molecule is rotated by a certain minimum angle (of $2\pi/n$), then it appears just as before the rotation. This axis is a n- fold axis and is represented by C_n .

A.1. Rotations as we know is a proper transformations and the right-hand-axis remains right handed and left remains left. But reflection is not so, as a result it is improper transformation. We will understand that later in lie group part

36 Molecular Symmetry

It is pretty clear that $C_n^n = e$. For our example $C_3^3 = e$ and our red axis is the 3-fold axis.

Also, $C_n^{n-1} = (C_n)^{-1}$, this shows that $C_n^k C_n^{n-k} = e$. So, C_n^k is the inverse of C_n^{n-k} .

It is possible that for a molecule, there are more than one axis of symmetry. In that case, the axis with maximum n is called the "Principle axis of Symmetry". Can you think of any example?

Most of the times for simplicity, we use z-aixs as our principle axis, i.e., we just rotate our molecule according to that. If in some case, we have a 2-fold symmetry axis perpendicular to the principle axis of symmetry, then the 2-fold symmetry axis is represented by \mathfrak{U}_2 . As an example, see the figure below.

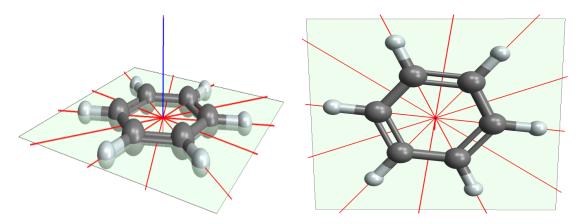


Figure A.2. Benzene axis of symmetry

As, we can clearly see the blue axis is the 6-fold symmetry axis and red ones are 2-fold symmetry axis. So, those are \mathfrak{U}_2 axises.

Let's see another molecule for more visual idea. Can you see which axis are what fold?

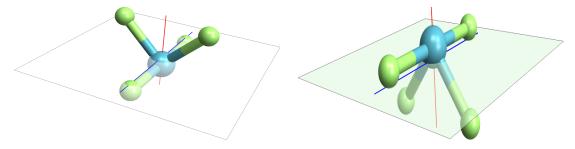


Figure A.3. Square Planar Xenon Tetrafluoride(XeF₄) axis of symmetry

Molecules can sometimes also have some $plane\ of\ symmetry$ (not like your non-symmetric face or mine).

Definition A.2: Plane of Symmetry

Planes with respect to which when some molecule is reflections is indistinguishable from it's original configuration are called *Plane of Symmetry*.

A plane which contains the principle axis of symmetry is called **vertical plane** and reflection w.r.t that plane is represented by σ_v .

A plane perpendicular to the axis of symmetry is called **horizontal plane** and reflection w.r.t that plane is represented by σ_h .

Sometimes, as in case of symmetry of a cube, diagonal planes of symmetry exist, for which we use the symbol σ_d . Let's see some examples:

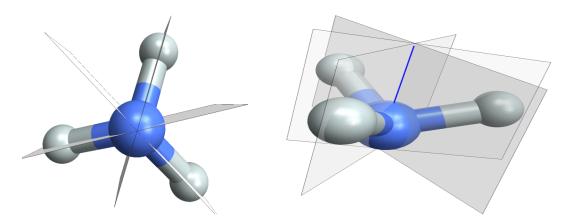


Figure A.4. Ammonia(NH₃) plane of symmetry $(3\sigma_v)$

Let's see another example for σ_v and σ_d using Xenon Oxytetrafluoride(XeOF₄).

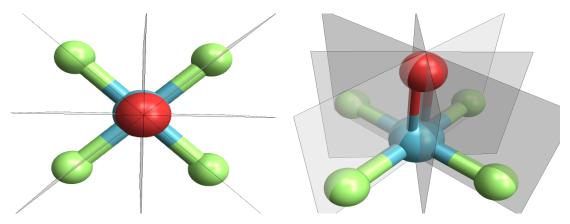


Figure A.5. Xenon Oxytetrafluoride(XeOF₄) with plane of symmetry (σ_v and σ_d).

The left figure above shows a very clear picture. Suppose, we put the molecule inside a square. All the fluorines are at each corner. The diagonal are exactly diagonal planes and reflection w.r.t them are σ_d and other two planes are σ_v .

It can be clearly seen,

$$\sigma_{v}^{2} = \sigma_{h}^{2} = \sigma_{d}^{2} = e \tag{A.1}$$

This is the case as it's basically reflection.

Aside these two, we can actually combine *rotation* and *reflection*. These are called *Roto-Reflection Symmetry*.

(Definition A.3: Roto-Reflection Symmetry)

If for a molecule, there is a σ_h plane (perpendicular to C_n axis), then a **roto-reflection** transformation S_n is either a rotation (C_n) followed by σ_h reflection or in the reverse order.

$$S_n = C_n \sigma_h = \sigma_h C_n \tag{A.2}$$

The molecule does not superimpose with the original molecule after the rotation. Achieving superposition requires the second step which is the reflection at a mirror plane that stands perpendicular to the improper axis. Only after the second step the operation is complete and we get the symmetry. It can be easily seen that the order in which C_n and σ_n are carried out is immaterial.

A important point to remember is that if n is odd integer, then n consecutive roto-reflections on the molecule would just be equivalent to a reflection in the horizontal plane, i.e.,

$$S_n^n = (C_n \sigma_h)^n = C_n^n \sigma_h^n = \sigma_h \tag{A.3}$$

So, only if n is even, then S_n is actually a distinct element (or else it will be simply σ_h).

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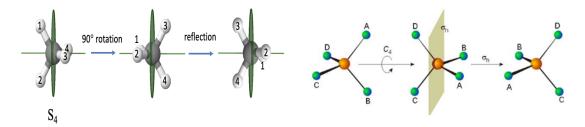


Figure A.6. Roto-Reflection Symmetry (Note: I have numbered the molecules).

A molecule also sometimes have another type of symmetry called "Inversion Symmetry" (C_i) . This happens if the molecule has a "point of symmetry". The symmetry element associated with an inversion, is the inversion center, also called "Center of Symmetry" (it is a single point).

When an inversion operation is performed, then each point of the object is moved through the inversion center to the other side. Each coordinate in the object (x, y, z) is inverted into the coordinates (-x, -y, -z). As an example see the figure below(for SF₆):

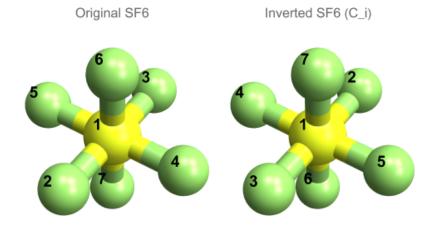


Figure A.7. C_i (Inversion) for the SF₆ molecule.

The property of such a point is that all the atoms of the molecules lie on lines passing through the center of symmetry, i.e, from 1 if we draw straight lines, all atoms lie on them.

It can be easily seen that $C_i^2 = e$ (again a basic property of inversion).

Sometimes, rather than drawing in 3D, we use another notion. This is shown below.

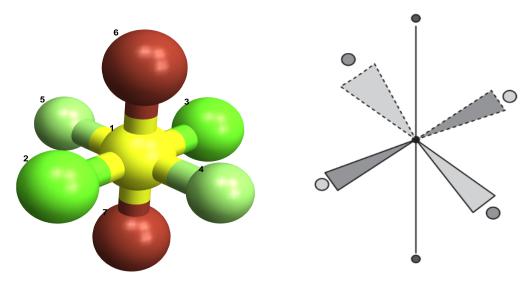


Figure A.8. 2D plotting of the 3D diagram

As we can clearly see, the brown atoms are represented by the up and down lines. Again, the light green atoms are represented by lightly shaded regions. The dashed lines represent going into the screen and the solid lines represent coming out of the screen. Similar for bright green coloured atom and dark shaded region.

A.2 Forging the Symmetry Group of a Molecule

A molecule may have one or more of the symmetry elements depending on it's structure. Once all of those are found, we can compose them in many ways and generate all possible symmetries of the molecule. As an example, suppose we have a molecule with 3-fold symmetry axis and a horizontal plane of symmetry.

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abelian group	invariant subgroup	
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conjugacy class ?	normal subgroup	•
coset	representation	ļ
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