Quantum Physics II

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Chapter 1

Recap of the basics

Introduction to quantum courses often start by describing the behavior of different quantum systems on a case by case basis. You consider a particle in a box, you consider a spin, you consider an atom, you consider a photon, etc. However, quantum systems of very different sorts can behave in similar ways by virtue of simply being quantum systems. With this line of thought, it can be powerful to abstract away from the actual stuff the system is made out of and just consider an N level quantum system (or a collection of M different N level quantum systems). This approach is aesthetically satisfying and also powerful in that it allows one to derive general results on what can/cannot be done with any quantum system (rather than a particular realisation of one). We will take this approach below to recap some of the basic principles of quantum mechanics.

1.1 The qubit

A two-level quantum system, also known as a quantum bit or "qubit", is the simplest possible quantum system. There are many different (approximate) physical realisations of a qubit in practise. Essentially, any physical system that is completely characterized by two states (or by a system with two energy states sufficiently separated from all others). Examples include:

1. An electron's spin ($|\uparrow\rangle$, $|\downarrow\rangle$)
2. A photon's polarization ($|H\rangle$, $|V\rangle$)
3. A pair of atomic (or molecular) levels ($|G\rangle$, $|E\rangle$)
4. The collective state of a super-current in a superconductor ($|G\rangle$, $|E\rangle$)
5. Two different arms a photon can take in an optical circuit ($|\text{'left'}\rangle$, $|\text{'right'}\rangle$)
6. ...

We abstract away from the different realisations and choose a canonical basis denoted by $\{|0\rangle, |1\rangle\} \equiv \mathcal{H}_1$.

A general single qubit state can be written as

$$|\Psi\rangle = \alpha\,|0\rangle + \beta\,|1\rangle\,, \;\; \alpha, \beta \in \mathbb{C}$$

with $|\alpha|^2 + |\beta|^2 = 1$. However, a more insightful representation of a single qubit $|\psi\rangle$ can be found by rewriting the constraint as

$$|\psi\rangle = \cos(\theta/2)\,|0\rangle \; + \; e^{i\phi}\sin(\theta/2)\,|1\rangle \tag{1.1}$$

Here $\cos(\theta/2)$ and $\sin(\theta/2)$ allow for arbitrary $|\alpha|$ and $|\beta|$ such that the state is normalized to 1[1], and ϕ allows for an arbitrary phase difference between $|0\rangle$ and $|1\rangle$. We note that the global phase is unphysical and so does not need to be considered for full generality. The parameters $\{\theta, \phi\}$ can be viewed as defining a unit vector in $\mathbb{R}^3$ in spherical coordinates,

$$\mathbf{v} = (\sin\theta\cos\phi,\ \sin\theta\sin\phi,\ \cos\theta)\,. \tag{1.2}$$

This observation is helpful as it allows one to visualise the state of a single qubit on what is known as the Bloch sphere as sketched in Fig. 1.1. For example, the $|0\rangle$ state corresponds to $\theta = 0$ and the $|+\rangle := \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ state corresponds to $\theta = \pi/2$ and $\phi = 0$. (We will come back to the Bloch sphere to study in more detail once we have covered density matrices in a couple of Chapters time.)

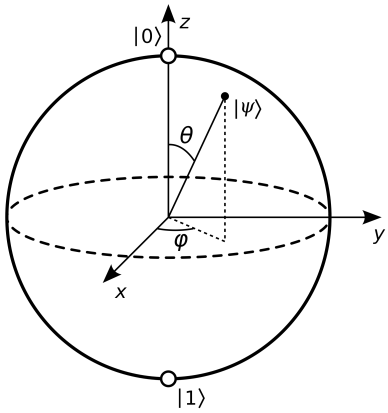


Figure 1.1: **The Bloch Sphere.** The state of a qubit can be represented as a vector in $\mathbb{R}^3$. (Image from Wikipedia).

Notice the analogy between classical computing bits and qubits. A qubit can be viewed as a generalization of a classical bit, which instead of being restricted to just 0 or 1, can take a superposition of 0 and 1. This perspective is crucial when it comes to discussing the potential of quantum systems for computation or communication. However, we stress that the abstract notion of a qubit is not only relevant in a quantum computational context but is a powerful approach to take more generally.

1.2 Multi-particle systems

We recall that given any two quantum systems $|\psi_A\rangle$ and $|\psi_B\rangle$ we denote their joint system via the tensor product $|\psi_A\rangle \otimes |\psi_B\rangle \equiv |\psi_A \psi_B\rangle$. Similarly, one can construct multi-qubit states. For n qubits, the space is given by

$$\mathcal{H}_n = \underbrace{\mathcal{H}_1 \otimes \cdots \otimes \mathcal{H}_1}_{n \text{ times}}$$

For two qubits, for example, the space is then

$$\mathcal{H}_2 = \{|0\rangle \otimes |0\rangle,\ |0\rangle \otimes |1\rangle,\ |1\rangle \otimes |0\rangle,\ |1\rangle \otimes |1\rangle\} = \{|00\rangle,\ |01\rangle,\ |10\rangle,\ |11\rangle\}$$

[1] You might be wondering why we have $\theta/2$ rather than just θ here. There are multiple levels of explanation for this factor which we will see as the course progresses. Firstly, it arises naturally in the density matrix formalism due to the fact that the trace of the square of a Pauli matrix is 2 not 2. More fundamentally, it arises from the relationship between the groups $SU(2)$ and $SO(3)$. For now, we just take it as part of the definition.

and the state of these two qubits is given by

$$|\Psi\rangle = \alpha|00\rangle + \beta|01\rangle + \gamma|10\rangle + \delta|11\rangle, \ \alpha,\beta,\gamma,\delta \in \mathbb{C}$$

with $|\alpha|^2 + |\beta|^2 + |\gamma|^2 + |\delta|^2 = 1$. One can also choose to consider this system as four level system of the form

$$|\Psi\rangle = \sum_{k=0}^{3} \alpha_k |k\rangle$$

where we have used the relabelling $|ij\rangle \to |i2^1 + j2^0\rangle$, i.e. $|00\rangle = |0\rangle, |01\rangle = |1\rangle, |10\rangle = |2\rangle, |11\rangle = |3\rangle$[2].

A system of n qubits corresponds to a $d = 2^n$ dimensional quantum system. One can also consider a d dimensional quantum system directly (without being restricted to a power of 2 dimensional system). A three level quantum system is known as a qutrit and higher dimensional systems are sometimes known as qudits.

1.3 Evolution

The evolution of a quantum state is given by the Schrodinger equation[3],

$$i\frac{\partial|\psi(t)\rangle}{\partial t} = H|\psi(t)\rangle. \tag{1.3}$$

When the Hamiltonian H is time-independent, the evolving state can be written directly as

$$|\psi(t)\rangle = U(t)|\psi(0)\rangle \tag{1.4}$$

where $U(t) \equiv e^{-iHt}$ is the *unitary time evolution operator*. While these two perspectives are equivalent and any unitary operation is generated by exponentiation of a Hamiltonian (i.e. a Hermitian operator) it is often convenient to abstract away and forget about the underlying Hamiltonian[4].

A unitary operation is a matrix U such that $UU^\dagger = U^\dagger U = \mathbb{I}$. Here are some important properties of unitary operations:

- **Reversible:** $U^\dagger(U|\psi\rangle) = |\psi\rangle$
- **Length preserving:** $\langle\psi|U^\dagger U|\psi\rangle = \langle\psi|\psi\rangle = 1$.
- **Linear:** $U(\alpha|\psi\rangle + \beta|\phi\rangle) = \alpha U|\psi\rangle + \beta U|\phi\rangle$.

Let us have a look at the evolution of a single qubit state. An important set of operators in this case are the Pauli matrices (for which there are a numerous notational conventions[5]):

$$\sigma_0 = \mathbb{I} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \ \sigma_1 = \sigma_x = X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \ \sigma_2 = \sigma_y = Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \ \sigma_3 = \sigma_z = Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{1.5}$$

Pauli matrices appear everywhere so it is helpful to become very familiar with their properties. Here are some useful (interrelated) properties that it is good to remember to save yourself needing to re-derive:

[2] I will switch freely between the notation $|i\rangle \otimes |j\rangle \equiv |ij\rangle \equiv |i2^1 + j2^0\rangle$ - while potentially a little confusing at first this is standardly done so you'll need to get used to it :)

[3] Here and through out these notes I will set $\hbar = 1$.

[4] At least until it comes to the symmetry properties of states. We will discuss again the relationship between these two pictures when we discuss Lie groups and Lie algebras in the groups and representations part of the course

[5] Again, I may switch between these various choices in notation as is standardly done.

1. $\mathrm{Tr}[\mathbb{I}] = 2$ and $\mathrm{Tr}[X] = \mathrm{Tr}[Y] = \mathrm{Tr}[Z] = 0$
2. For $i = 1, 2, 3$ we have $\sigma_i \sigma_j = \delta_{ij}\mathbb{I} + i\epsilon_{ijk}\sigma_k$ where ϵ_{ijk} is the Levi-Civita symbol (i.e. $\sigma_i^2 = \mathbb{I}$, $\sigma_x\sigma_y = i\sigma_z$, $\sigma_y\sigma_x = -i\sigma_z$, ...)
3. Commutation: $[\sigma_i, \sigma_j] = 2i\epsilon_{ijk}\sigma_k$
4. Anticommutation: For $i = 1, 2, 3$ we have $\{\sigma_i, \sigma_j\} = 2\delta_{ij}\mathbb{I}$.
5. The Pauli matrices form an orthonormal basis with $\mathrm{Tr}[\sigma_i\sigma_j] = 2\delta_{ij}$

Exercise: verify these identities!

Pauli matrices are both hermitian and unitary so, depending on the context, they can be thought of as: evolution operators, generators of evolution operators or as measurement. In fact being able to switch freely between these perspectives is very convenient.

Paulis as gates: For example, X acts as the NOT gate on a quantum bit:

$$\begin{aligned} X\,|0\rangle &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} = |1\rangle \\ X\,|1\rangle &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = |0\rangle\,. \end{aligned} \tag{1.6}$$

Exercise: compute the action of each of the Pauli operators on the Bloch vector of a generic single qubit state.

Paulis as generators. A Pauli operator can also be seen as a generator of a unitary evolution. To see this recall that the Pauli matrices form a matrix basis. As such, any single qubit Hamiltonian can be written as[6]

$$H = \sum_{i=1}^{3} \omega n_i \sigma_i = \omega \mathbf{n}.\boldsymbol{\sigma}\,, \tag{1.7}$$

where we have defined the vectors $\mathbf{n} = (n_1, n_2, n_3)$, $\boldsymbol{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ and we have pulled out a factor ω as setting the over all energy scale. It follows that any single qubit unitary can be written as

$$U = e^{-iHt} = e^{-i\omega\mathbf{n}.\boldsymbol{\sigma}t}\,. \tag{1.8}$$

What is the effect of applying this to a generic single qubit state $|\psi\rangle = \cos(\theta/2)\,|0\rangle + e^{i\phi}\sin(\theta/2)\,|1\rangle$? To see this we first note you can use the properties of the Pauli operators combined with the definition of the matrix exponential (*Exercise: do this!*) to show that:

$$e^{-i\mathbf{n}.\boldsymbol{\sigma}\omega t} = \cos(\omega t)\mathbb{I} - i\sin(\omega t)\mathbf{n}.\boldsymbol{\sigma}\,. \tag{1.9}$$

It now remains to evaluate the effect of this operator on a single qubit state. Let us look at an example. Suppose $\mathbf{n} = \mathbf{n_z} = (0, 0, 1)$ then $\mathbf{n_z}.\boldsymbol{\sigma} = \sigma_z$ and we have

$$\begin{aligned} e^{-i\omega\sigma_z t}(\cos(\theta/2)\,|0\rangle \,+\, e^{i\phi}\sin(\theta/2)\,|1\rangle) &= \cos(\theta/2)e^{-i\omega t}|0\rangle + \sin(\theta/2)e^{i\phi}e^{+i\omega t}|1\rangle \\ &= e^{-i\omega t}(\cos(\theta/2)|0\rangle + \sin(\theta/2)e^{i(2\omega t+\phi)}|1\rangle) \end{aligned} \tag{1.10}$$

[6]We have dropped the identity term here as it will only generate a global phase and so is unphysical if considering just the evolution of a single qubit. Note that if we were considering the partial evolution of a two qubit system we would need to be more careful as this could be a (physical) relative phase.

Recalling the Bloch vector in Eq. (1.2) we thus see that the state rotates around the Z axis by an angle $2\omega t$.

In fact this holds true more generally - a Hamiltonian of the form Eq. (1.7) causes a qubit state to rotate around the axis $\mathbf{n}$ at a rate $2\omega t$ as shown in Fig. 1.2. *Exercise: show this!* This provides a convenient means of inspecting how a single qubit state will evolve without needing to perform explicit calculations.

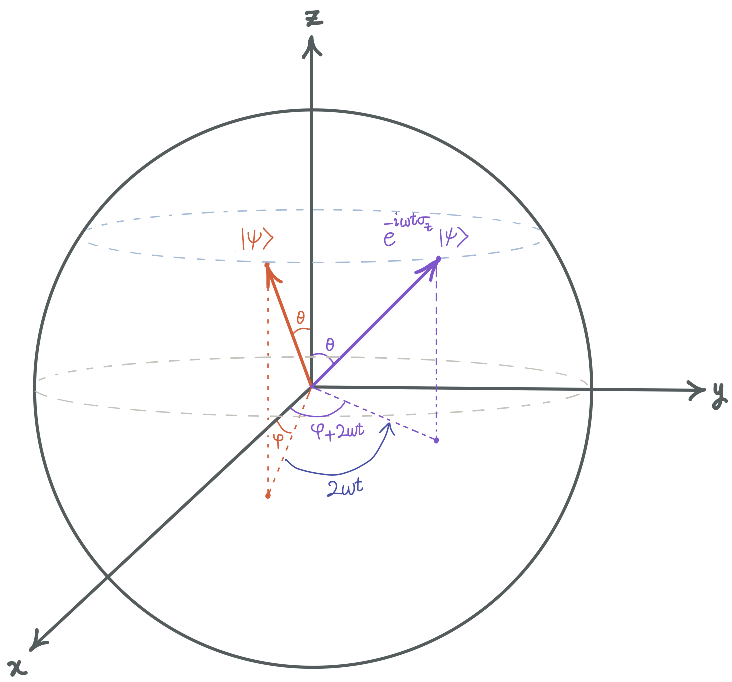


Figure 1.2: **The Rotation in Bloch Sphere.** Pauli matrices can be a generator of a rotation.

1.4 Measurements

There are multiple ways of representing measurements in quantum mechanics. The first measurement that students usually are introduced to are 'observables'. These are Hermitian operators, i.e. an operator M such that $M = M^\dagger$. In virtue of being Hermitian, observables are diagonalizable and have real eigenvalues so we can write

$$M = \sum_k \lambda_k |\lambda_k\rangle\langle\lambda_k| \,. \tag{1.11}$$

The expectation of an observable M in a state $|\psi\rangle$ is then given by

$$\langle M\rangle = \langle\psi| M |\psi\rangle = \sum_k \lambda_k p_k \tag{1.12}$$

with $p_k = |\langle\lambda_k|\psi\rangle|^2$.

The operator $|\lambda_k\rangle\langle\lambda_k|$ is alternatively known as a projector. We can also directly define measurements in terms of a set of projectors $\{\Pi_k\}$ where $\Pi_k^2 = \Pi_k$. The probability of obtaining an outcome k is given by

$$p_k = \langle\psi| \Pi_k |\psi\rangle \tag{1.13}$$

and so to ensure that the probabilities sum to 1 we require that $\sum_k \Pi_k = 1$.

In the case of rank 1 projector (i.e. those that have only eigenvalues 1 and 0) we can always write $\Pi_k = |\lambda_k\rangle\langle\lambda_k|$ for some $|\lambda_k\rangle$. However, this not always be the case. Sums of orthogonal projectors are also orthogonal projectors but will not be rank one, e.g.

$$\Pi_{\text{even}} = |00\rangle\langle 00| + |11\rangle\langle 11| \ , \ \ \Pi_{\text{odd}} = |01\rangle\langle 01| + |10\rangle\langle 10| \,. \tag{1.14}$$

In the case of an 'ideal' measurement it is commonly said that the state of the system 'collapses' onto the state

$$\frac{\Pi_k|\psi_k\rangle}{\sqrt{p_k}}, . \tag{1.15}$$

This captures the idea that ideal measurements are repeatable because another instantaneous measurement would give the same outcome and leave the output state unchanged. In the case of rank one measurements the resulting state is simply the eigenstate corresponding to the measured outcome. That is, if one obtains outcome k where $\Pi_k = |\lambda_k\rangle\langle\lambda_k|$, the resulting state on the system is $|\lambda_k\rangle$.

It is worth noting that this account of measurement is not the full story. Firstly, it is not sufficiently general and there are all sorts of measurements that cannot be captured by observables or projectors (e.g. imperfect measurements). Instead, a complete account of measurement can be provided by the positive operator-valued measure (POVM) formalism. This goes beyond the requirements of this course but is covered in my Quantum Information Theory course and Jean-Philippe Brantut's Quantum optics course if you are interested in learning more. Secondly, the claim that the quantum state collapses on measurement is utterly baffling for a number of reasons. This we will return to in Chapter 6.

Chapter 2

What makes quantum different?

For most people, the formalism of quantum mechanics (when first introduced to it at least) is so different to most of the physics you have seen before that it is hard to dissect what about quantum physics really is different from classical physics, versus what is just foreign notation. This can partially be addressed by familiarity - hopefully you are already relatively comfortable with the quantum formalism[1] but part of the aim of this course is to get you more and more fluent at working with quantum mechanics.

Once you are well acquainted with the quantum formalism, the opposite problem can occur. It's easy to become so used to working with it that you forget to take a step back and take in quite how weird and wonderful it is. And it is important to understand how quantum mechanics is special, not just because it's fun and explaining it is a great trick at parties, but also because it's only by understanding what makes quantum physics special that we can better learn how to manipulate quantum systems to our advantage. This insight is at the heart of what is sometimes called the 'second quantum revolution' that is currently underway - where increasingly we are able to manipulate quantum systems for technological advantages.

This chapter will take a two pronged approach to trying to highlight what makes quantum mechanics unique. Firstly, we will present a theories of (thought[2]) experiments. In parallel, we will present a series of no-go theorems about what is possible and not possible in a quantum world. This chapter will heavily draw on Terry Rudolph's Quantum Physics lecture notes from when he was a professor at Imperial College London.

2.1 Superposition and Interference

The concept of a superposition is one that we are particularly vulnerable to forgetting is mysterious due to over familiarity. The following (thought) experiments are intended to try and reignite an appreciation for some of the wonder of superpositions.

Imagine we have a quantum system that can be in two different states $|0\rangle$ and $|1\rangle$ and study its evolution in time. John Townsend in Chapter 1 of 'A Modern Approach to Quantum Mechanics' considers the Stern-Gerlach experiment with a particle that can bend to the left '0' or bend to the right '1'. Terry Rudolph makes the picture more exciting (but less realistic[3]) by talking about cats in the 'alive' state and 'dead' state. If you like atomic physics think about

[1] Seeing that classical mechanics at an advanced level can also be formalized in similar manner to quantum mechanics can also help one appreciate that its not quantum's formalism that makes it special. You will see this in the Analytical Mechanics course.

[2] While all of these 'experiments' are in some sense physically possible from a theorist's perspective just the thought of most of them would hurt many experimentalists.

[3] We end up with resuscitated zombie cats.

an atom that can be in a 'ground' state or 'excited' state. If you like photonics, think about the 'left' or 'right' arm of an interferometer. Take your pick. I'm going to channel my inner quantum information theorist and just call the two states '0' and '1'.

Thought experiment 1: We start with a system in state $|1\rangle$. We wait half an hour before measuring it. We then find that 50% of the time it is in state $|1\rangle$ and that 50% of the time it is in state $|0\rangle$.

Thought experiment 2: We start with a system in state $|0\rangle$. We wait half an hour before measuring it. We then find that 50% of the time it is in state $|1\rangle$ and that 50% of the time it is in state $|0\rangle$.

Thought experiment 3: We start with a system in state $|0\rangle$. We wait half an hour before measuring it. We then find that 50% of the time it is in state $|1\rangle$ and that 50% of the time it is in state $|0\rangle$. We then wait another half an hour before measuring again. What do we expect to find?

Well drawing a probability tree we expect to end up with a 50% chance of finding the system in state $|0\rangle$ or state $|1\rangle$ as shown in Fig. 2.1. Overall, half the time we end up with the system in state $|1\rangle$ and half the time we end up with the system in state $|0\rangle$.

Thought experiment 4: We start with a system in state $|0\rangle$. We wait a full hour before measuring it. What do we expect to find?

Well intuitively / thinking classically we would expect to see the same as in thought experiment 3. But when we do experiment 4 we actually find that the system is always in state $|0\rangle$. What is going on here? Well firstly, that the act of measuring the system seems to have an effect on how the system behaves. Secondly, the state of the system after half an hour is ***not*** that it is in either $|0\rangle$ ***or*** $|1\rangle$ with equal probability. Rather, that it is in a special quantum state - it is in a *superposition*.

Let us describe this situation mathematically. The dynamics of thought experiment one can be described as:

$$|1\rangle \rightarrow \frac{1}{2}(|1\rangle + |0\rangle)\,. \tag{2.1}$$

Thought experiment two can instead be described as

$$|0\rangle \rightarrow \frac{1}{2}(-|1\rangle + |0\rangle)\,. \tag{2.2}$$

The negative sign here is essential to account for the linearity of quantum mechanics (i.e. that its dynamics are governed by unitary operations) - this ensures that orthogonal states are mapped to orthogonal states. It follows from Eq. (2.1) and Eq. (2.2) and the linearity of quantum mechanics that the third thought experiment can be described as

$$|1\rangle \rightarrow \frac{1}{2}(|1\rangle + |0\rangle) \rightarrow \frac{1}{2}\left(\frac{1}{2}(|1\rangle + |0\rangle) + \frac{1}{2}(-|1\rangle + |0\rangle)\right) = |0\rangle\,. \tag{2.3}$$

The cancellation of the terms here is what is known as quantum *interference*. It is this causes the probability tree picture in Fig. 2.1 to break down and ensures that a quantum state of the form of Eq. (2.1) cannot be understood simply as describing a system that is in '0' or '1' with probability 1/2 each. Rather they represent a non-classical state of affairs, that we cannot described using our conventional classical vocabulary, and instead just call a 'superposition'.

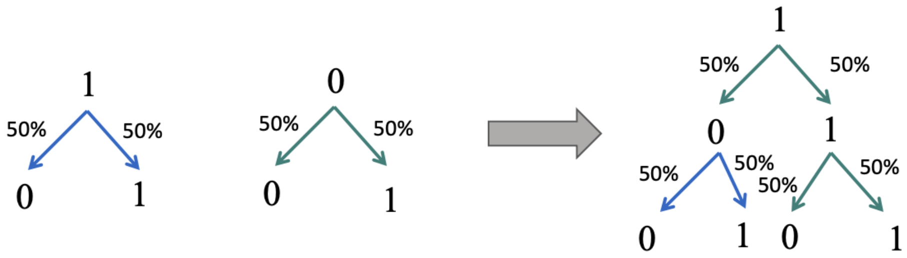


Figure 2.1: Probability tree diagram corresponding to thought experiments 1, 2 and 3 (from left to right)

2.2 The Quantum Eraser

The two slit experiment is often the first thought experiment a student encounters when studying quantum mechanics. Here we will explore some variants to it that highlight the curious interplay between coherence, interference and entanglement.

Standard two slit experiment (1): Let us start with the standard two slit experiment. We suppose that single horizontally polarized photons impinge on a screen with two slits and hit a second screen placed behind the first (see Fig. 2.2a)). Although the photons hit the screen one by one we see an interference pattern on the screen behind.

Standard two slit experiment (2): We now suppose that a 90 degrees polarisation shifter is placed behind one of the slits (so that the light coming through it now is vertically polarized) but otherwise leave the set up unchanged (Fig. 2.2b). *What happens this time?*

In this case the interference pattern does not arise. Instead we see a simple mixture of the two patterns we would get if the photons went either through the top or the bottom slit as shown in Fig. 2.2b. This is because if we measured each photons polarisation then we would be able to determine if it went through the top or the bottom slit. Even if we do not in fact check which slit we went through this information is enough to destroy the interference pattern.

Here is how to understand this mathematically. Let $\psi_1(x,t)$ be the wavefunction of a photon emerging from the first slit, and $\psi_2(x,t)$ be that from the second slit. Let the polarisation of a photon be labelled by a H (horizontal) or V (vertical) substate, so that a horizontally-polarised photon emerging from the first slit is written as $|\psi_1, H\rangle = |\psi_1\rangle \otimes |H\rangle$. In the original two slit experiment the state of the photon after going through the two slits is of the form

$$|\Psi(x,t)\rangle = \frac{1}{\sqrt{2}}(|\psi_1(x,t)\rangle + |\psi_2(x,t)\rangle) \otimes |H\rangle \tag{2.4}$$

and on measuring the position of the particle at the second screen we get the probability density

$$P(x) = \langle\Psi(x,t)|\,|x\rangle\langle x|\,|\Psi(x,t)\rangle = |\psi_1(x,t) + \psi_2(x,t)|^2/2\,. \tag{2.5}$$

In the second case the state of the photon after passing through the two slits and the polarization shifter is of the form

$$|\Phi(x,t)\rangle = \frac{1}{\sqrt{2}}(|\psi_1(x,t)\rangle \otimes |V\rangle + |\psi_2(x,t)\rangle \otimes |H\rangle) \tag{2.6}$$

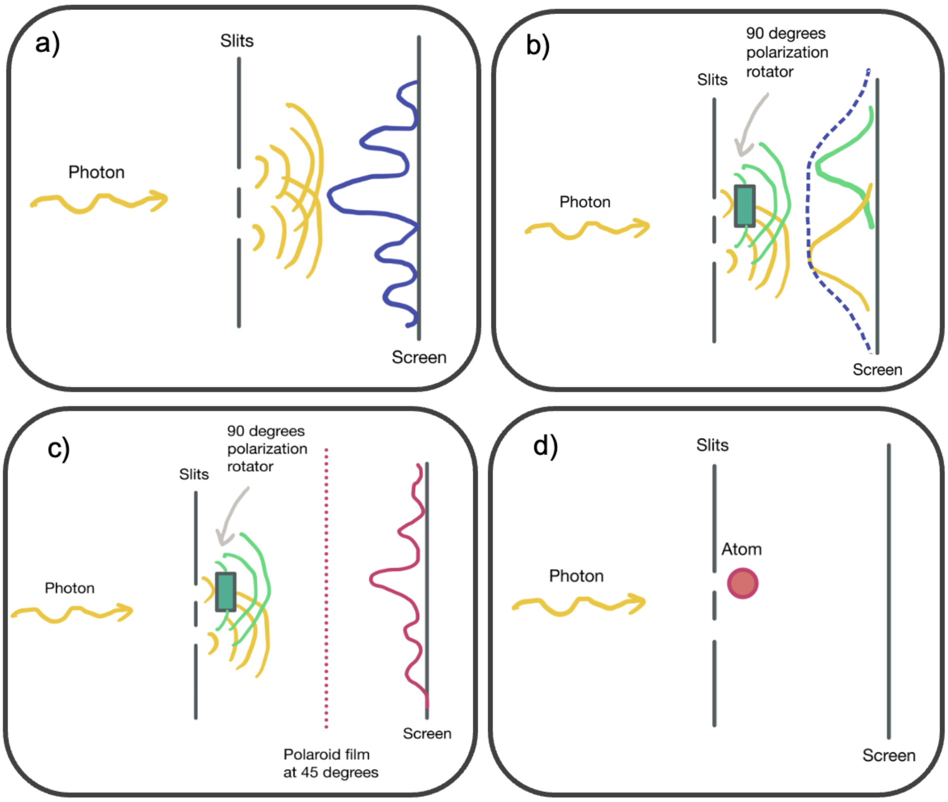


Figure 2.2: Quantum eraser experiments

and so the probability density function of the photons hitting the screen is

$$\begin{aligned} P(x) &= \langle\psi_1(x,t)|\,|x\rangle\langle x|\,|\psi_1(x,t)\rangle\langle V|V\rangle + \langle\psi_2(x,t)|\,|x\rangle\langle x|\,|\psi_2(x,t)\rangle\langle H|H\rangle \\ &= (|\psi_1(x,t)|^2 + |\psi_2(x,t)|^2)/2 \end{aligned} \tag{2.7}$$

Quantum eraser: We now suppose that as well as the 90 degrees polarisation shifter behind one of the slits we add a polaroid sheet at 45 degrees, which only outputs light in the state $|\nearrow\rangle = \frac{1}{\sqrt{2}}(|H\rangle + |V\rangle)$. This is shown in Fig. 2.2c). *What happens this time?*

We see the interference pattern again but at half the intensity. Why? The light coming through the top slit is vertically polarized and the photons coming through the bottom slit is horizontally polarized. The polaroid sheet effectively measures the polarization degree of freedom in the $\{|\nearrow\rangle, |\swarrow\rangle\}$ basis and only lets through measurement outcomes that project the light to $|\nearrow\rangle$. Now both H and V photons have a 50% chance of being measured to be $|\nearrow\rangle$ and so the sheet lets through only half the photons. But crucially all the photons (both the ones from the upper slit and the lower slit) that get let through are in the $|\nearrow\rangle$ state and so it's impossible to determine which slit any photon went through.

Exercise: What changes if the polaroid sheet only lets through $|\swarrow\rangle = \frac{1}{\sqrt{2}}(|H\rangle - |V\rangle)$ photons?

Delayed quantum eraser: Let's go back to the simple two slit experiment and this time place an atom behind one of the slits as sketched in Fig. 2.2d). Now this would be hard to arrange in practise but let us suppose that the photon that passes the atom flips the spin of an outer electron from $|\downarrow\rangle$ to $|\uparrow\rangle$ but is not absorbed[4]. (For each photon that we send through the two slit experiment we use a new atom and store the previous in a quantum memory). What happens in this case?

Well it depends on the basis that the atom is measured in. If the atom is measured in basis $\{|\uparrow\rangle, |\downarrow\rangle\}$ then we end up with version 2 of the standard two slit experiment where we know which slit the photon went through. However, if we measure in the $\{|\nearrow\rangle, |\swarrow\rangle\}$ basis we end up with the quantum eraser version, and the interference reappears (but we do not lose half the photons this time). *Exercise: Work through the maths!*

The interference pattern depends on the basis that the atom is measured in - something we subjectively choose. And more puzzling still, this is true even if the atoms are taken far away before being measured! So a natural thought might be - can we use this to signal?

2.3 No signalling

Consider again the delayed quantum eraser thought experiment from the lectures and exercises last week. We saw the following.

- **Measure in the Z basis:**

  If we obtain $|\uparrow\rangle$ then the pattern is $|\psi_1(x,t)|^2$.
  If we obtain $|\downarrow\rangle$ then the pattern is $|\psi_2(x,t)|^2$.

- **Measure in the X basis:**

  If we obtain $|\nearrow\rangle$ then the interference pattern is $\frac{1}{2}|\psi_1(x,t) + \psi_2(x,t)|^2$.
  If we obtain $|\swarrow\rangle$ then the interference pattern is $\frac{1}{2}|\psi_1(x,t) - \psi_2(x,t)|^2$.

Could we try and use this setup for a superluminal signal? On the surface it might look like we should be able to. Suppose Alice and Bob try and signal using the code that an interference pattern corresponds to the bit '0' and no interference corresponds to the bit '1'. Then Bob it would seem could measure Z or X to send '0' or '1' to Alice and this would be true no matter how far away he is from Alice, seemingly allowing superluminal signalling. However, if Bob could signal to Alice in this way it would violate special relativity. So what breaks down?

Well the key thing to note is that the interference pattern depends on not just the measurement, but the measurement *outcome*. Say the atom is measured in the Z basis. Bob will obtain $|\uparrow\rangle$ and $|\downarrow\rangle$ with equal probabilities (because the photon is equally likely to go through either slits) and so the resulting pattern on the screen is

$$p(x) = |\psi_1(x,t)|^2 + |\psi_2(x,t)|^2 . \tag{2.8}$$

Similarly, if Bob measures in the X basis then the states $|+\rangle$ and $|-\rangle$ are obtained with equal probabilities and so the resulting pattern is

$$p(x) = |\psi_1(x,t) + \psi_2(x,t)|^2 + |\psi_1(x,t) - \psi_2(x,t)|^2 = |\psi_1(x,t)|^2 + |\psi_2(x,t)|^2 . \tag{2.9}$$

That is, the pattern is the same in either case!

[4]An experiment of this spirit but not of this exact form has been conducted. Take a look at the wikipedia page on the delayed quantum eraser to learn more.

In order to be able to communicate with this set up Bob would need to tell Alice for each photon that went through the setup which outcome he obtained. She could then mark the photons according to the outcome obtained and determine whether or not an interference pattern was observed for measurement outcomes of the same sort (corresponding to X measurement) or no interference pattern (corresponding to Z measurement). However, this requires communication which defeats the purpose of the purported signalling protocol.

Ok, so this quantum erasor protocol doesn't work. Could another more general protocol work? Suppose Alice and Bob share two halves of generic entangled state $|\Psi\rangle$ that they want to use to try and signal. Suppose Bob considers two different measurements Π_0 and Π_1 that he wants to use to signal '0' or '1' respectively. Let us suppose that these measurements collapse Alice's state as follows.

1. **Bob measures Π_0:** Alice obtains the states $|\psi_i\rangle$ with probability p_i.

2. **Bob measures Π_1:** Alice obtains the states $|\phi_i\rangle$ with probability q_i.

Then in order for Alice to be able to tell whether Bob measured Π_0 or Π_1 she will need to be able to find a measurement Π_A such that

$$\sum_i p_i \langle\psi_i| \Pi_A |\psi_i\rangle \neq \sum_i q_i \langle\phi_i| \Pi_A |\phi_i\rangle . \tag{2.10}$$

It turns out that it is impossible to find such an operator. That is, for any choice in Π_A the above expression is an equality. It follows that it is impossible to use an entangled state faster than the speed of light. For an example of this see this chapter's problem sheet. We will also demonstrate this more rigorously when we cover reduced states in a few lectures time.

2.4 Non-locality and Bell inequalities

In this section we will explore how quantum entanglement can produce correlations that cannot be explained by classical observers that pre-share classical correlated data/randomness. More concretely, we will see how Bell's theorem, and experimental verifications of it, imply that not only quantum physics but also our world is inherently 'non-local'. I will start this section with an unconventional way of framing the Bell's Theorem that I have shamelessly borrowed from Terry Rudolph.

2.4.1 Quantum Psychics

Suppose there were two friends Alice and Bob who claimed to share a psychic connection. How could you go about testing it? Let's put Alice and Bob into isolated rooms with no way they can pass any messages between them. Outside Alice's room is a sceptic, let's call him Spock, who tosses a coin and tells Alice the outcome. Outside Bob's room is another sceptic, Kirk, who similarly tosses a coin and tells Bob the outcome. Alice and Bob must then respond with either yes 'Y' or no 'N'. What can Spock and Kirk ask Alice and Bob to do to try to determine if they are psychic? They consider the following tests...

Test 1: *Every time Alice and Bob get told the same coin outcome they must give the same answer, every time they get different outcomes they must give different answers.*

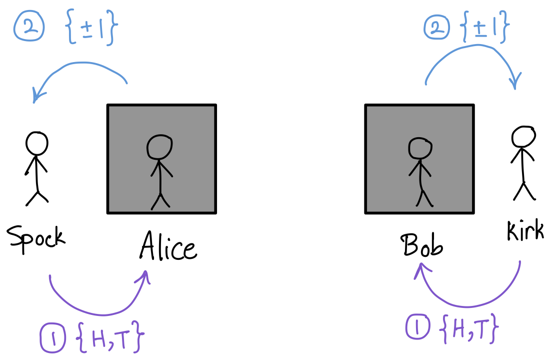


Figure 2.3: **The Quantum Psychics Game.**

This clearly is a flawed test. Alice and Bob can pass it simply by deciding in advance that they will both say yes to heads and no to tails.

Realising this, the Spock and Kirk instead toy with proposing an alternative test...

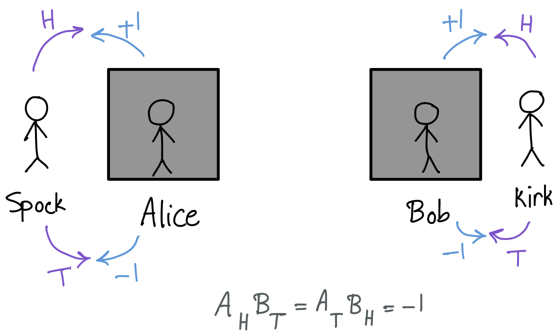


Figure 2.4: **The Quantum Psychics Game: Test 1.**

Test 2: *Every time Alice and Bob get told the same coin outcome they must give opposite answers, every time they get different flips they must give the same answers.*

On further thought this test is equally flawed. Alice and Bob agree in advance that they will give different outcomes. That is, Alice says yes to heads and no to tails but Bob does the converse.

Instead the Spock and Kirk propose the following test.

Test 3: *Every time Alice and Bob get told 'H' they must give opposite answers, but otherwise they must give the same answer.*

Now if you play around with this you'll see that there is no strategy that Alice and Bob can cook up in advance in order to fool the sceptics. Try this! After playing with a few examples, the easiest way to definitively prove it to yourself is to represent the binary answers 'Y' and 'N' by +1 and -1 respectively. Then the rules of the game can be formalized as trying to find an

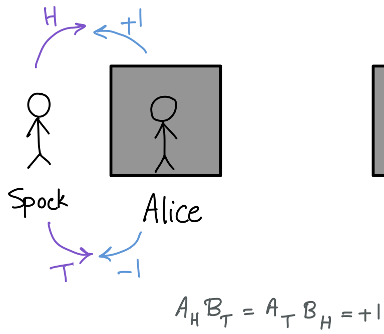


Figure 2.5: **The Quantum Psychics Game: Test 2.**

assignment of A_H, A_T, B_H and B_T such that

$$\begin{aligned} A_H B_H &= -1 \\ A_H B_T &= 1 \\ A_T B_H &= 1 \\ A_T B_T &= 1 \end{aligned} \tag{2.11}$$

Multiplying the left hand side of these four equations together gives $A_H^2 A_T^2 B_H^2 B_T^2 = 1$. However, multiplying the right hand side together gives -1. Hence there cannot be an assignment of A_H and B_H that satisfies all the rules of the test and as such this test is a viable means to testing if Alice and Bob are psychic.

In fact, the maximum number of rules that can be satisfied in Eq. 2.11 for any strategy taken by Alice and Bob is 3. (Convince yourself of this!) That is, at best Alice and Bob can pick a strategy that will lead to them fooling the sceptics for 3 out of the 4 possible coin toss combinations:

$$P_{\text{win}} \leq 3/4 \,. \tag{2.12}$$

This is an example of a Bell inequality. If Alice and Bob reliably can win with a probability significantly greater than 3/4 then it would seem reasonable to assume that they really are psychic.

However, if Alice and Bob share entangled Bell states, $|\phi^+\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$, then they can use the non-classical correlations stored in the Bell state to pass the sceptics test. Alice and Bob's strategy to do so is as follows.

- If Alice gets told 'H' she measures in the Z basis and says 'Y' if she gets '$|0\rangle$' and 'N' if she gets '$|1\rangle$'.
- If Alice gets told 'T' she measures in the X basis and says 'Y' if she gets '$|+\rangle$' and 'N' if she gets '$|-\rangle$'.
- If Bob gets told 'H' he measures in the basis

$$\left\{|h\rangle = \sin(\pi/8)|0\rangle + \cos(\pi/8)|1\rangle \,,\, |\bar{h}\rangle = \cos(\pi/8)|0\rangle - \sin(\pi/8)|1\rangle\right\} \tag{2.13}$$

  and says 'Y' if he gets '$|h\rangle$' and 'N' if she gets '$|\bar{h}\rangle$'.
- If Bob gets told 'T' he measures in the basis

$$\left\{|t\rangle = \cos(\pi/8)|0\rangle + \sin(\pi/8)|1\rangle \,,\, |\bar{t}\rangle = \sin(\pi/8)|0\rangle - \cos(\pi/8)|1\rangle\right\} \tag{2.14}$$

and says 'Y' if he gets '$|t\rangle$' and 'N' if she gets '$|\bar{t}\rangle$'.

Alice and Bob can beat test 3 with probability

$$P_{\text{Quantum}} = \cos(\pi/8)^2 = \frac{2+\sqrt{2}}{4} \approx 0.854\,. \tag{2.15}$$

Exercise: Check this!

However, crucially this is an intriguing form of telepathy. They can use it to cheat the sceptics test but (as we saw before and you will see in the problem sheet) they cannot use it to signal. So is it useful for anything? In fact, it proves useful in quantum cryptography (but that is beyond the remit of this course).

Terry's quantum psychics version of the Bell inequality is entirely equivalent to a more conventional framing of the Bell's theorem known as the CHSH inequality. Rather than asking what is the probability of Alice and Bob winning test 3, the CHSH inequality is a bound on the sum of the expectation values of the product of Alice and Bob's answers for each of the different possible combinations of outcomes. That is, a bound on the correlation coefficient

$$C := \langle A_T B_T\rangle + \langle A_H B_T\rangle + \langle A_T B_H\rangle - \langle A_H B_H\rangle \tag{2.16}$$

where

$$\begin{aligned}\langle A_H B_H\rangle = (-1)\times P(A_H = 1, B_H = -1|H,H) + (-1)\times P(A_H = -1, B_H = 1|H,H)\\ +(+1)\times P(A_H = 1, B_H = 1|H,H) + (+1)\times P(A_H = -1, B_H = -1|H,H)\,.\end{aligned} \tag{2.17}$$

and similarly for the other expectations values. We want to relate this to probability of winning in test 3,

$$\begin{aligned}P_{\text{win}} = \frac{1}{4}\Big(&P(A_H = 1, B_H = -1|H,H) + P(A_H = -1, B_H = 1|H,H)\\ &P(A_H = 1, B_T = 1|H,T) + P(A_H = -1, B_T = -1|H,T)\\ &P(A_T = 1, B_H = 1|T,H) + P(A_T = -1, B_H = -1|T,H)\\ &P(A_T = 1, B_T = 1|T,T) + P(A_T = -1, B_T = -1|T,T)\Big)\end{aligned} \tag{2.18}$$

To do so, we note that as the probability of the different outcomes have to sum to 1, we can write $\langle A_H B_H\rangle$ as

$$\langle A_H B_H\rangle = 1 - 2(P(A_H = 1, B_H = -1|H,H) + P(A_H = -1, B_H = 1|H,H))\,. \tag{2.19}$$

On using a similar trick with the other expectations values, the probability of winning in test 3 is given by

$$P_{\text{win}} = \frac{1}{8}\left((1 - \langle A_H B_H\rangle) + (1 + \langle A_H B_T\rangle) + (1 + \langle A_T B_H\rangle) + (1 + \langle A_T B_T\rangle)\right) = \frac{1}{2} + \frac{1}{8}C\,. \tag{2.20}$$

As $P_{\text{win}} \le 3/4$, it follows that

$$C = 8\left(P_{\text{win}} - \frac{1}{2}\right) \le 2\,. \tag{2.21}$$

However for quantum players we have $P_{\text{quantum}} = \frac{1}{2} + \frac{\sqrt{2}}{4}$ and so

$$C_{\text{quantum}} = 2\sqrt{2}\,. \tag{2.22}$$

2.4.2 More formal derivation (i.e. pinning down exactly what exactly is spooky)

We introduced Bell inequalities above with a thought experiment about testing psychics. This hopefully helped to give you an intuition about what is so strange about violating a Bell inequality. Below we present a more formal derivation of the CHSH inequality that helps to pin down precisely how the correlations of a Bell inequality violating system are different to conventional classical correlations.

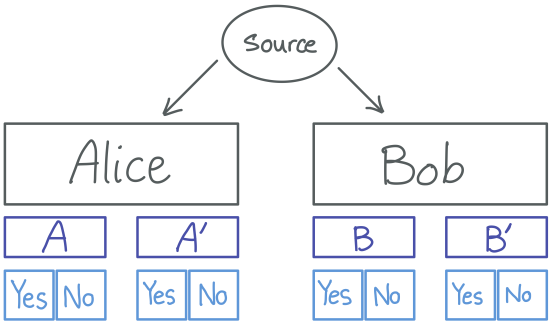


Figure 2.6: **The CHSH Inequality**

Consider a bipartite system where one part is sent to a LHS measuring device and the other to a RHS measuring device as sketched in Fig. 2.6. The LHS measuring device has a lever allowing it to measure either A or A'. The RHS measuring device can be set to B or B'. When a measurement is made the light under either "Yes" or "No" turns on. We are interested in the correlations between result combinations when measurements are made on the different settings.

Let the probabilities is different result combinations be written as $P(l,r|LR)$ where L and R are placeholders for the settings of the left and right measuring devices (i.e., L can take values A or A' and R values B and B') and l and r are placeholders for the results shown on the LHS and RHS measuring devices and as such can be either be"yes" or "no".

Bell inequalities define a correlation coefficient C as in Eq. (2.27) and then place an upper bound on possible values this coefficient can take if you assume "factorisability". **Factorisability** is the statement that the probability of l and r can be written as

$$p(l,r|LR) = \int P(l|L,\lambda)P(r|R,\lambda)P(\lambda)d\lambda\,. \tag{2.23}$$

What is the significance of the factorisability assumption? If events x and y are uncorrelated then their joint distribution can be written as $P(x,y) = P(x)P(y)$. Similarly, the statement: $P(x,y|\alpha,\beta,\gamma) = P(x|\alpha,\beta,\gamma)P(y|\alpha,\beta,\gamma)$ says that the probabilities of x and y are uncorrelated once you take into account variables α,β and γ. Put another way, factors α,β and γ are sufficient to explain any correlations in the probabilities of x and y. For example, it seems reasonable to expect that the probability that a pub sells more than 100 ice creams in a day, $P(x)$, is correlated of the probability that the pub sells more than 1000 pints of cider, $P(y)$, but these correlations can be explained by taking into account all the various common factors such as outside temperature (α), day of the week (β), and the number of important sporting fixtures that day (γ). The parameter λ is introduced to incorporate all such common factors[5] and giving the original statement of factorisability, Eq. (2.23).

[5]Note; λ only includes factors from the events shared histories, it does not include explicit information about the results of either x or y. My example above would not be factorisable if a pub had a rule that every time 25 ice creams were sold they would toss a coin to decide whether to sell any more ciders that day.

As such, the statement of "factorisability" used to set up the Bell inequality can be understood as follows. Given λ, the probability of the outcome of a particular measurement on the LHS given that A is measured, is uncorrelated to the probability of a particular result on the RHS, given that B is measured. That is, λ incorporates all effects from the system's shared history.

In terms of the experimental set up we are considering here λ represents all information concerning the initial state of the system and the experimental equipment before the system is divided and sent to the different measuring devices. As such, by denying that the joint probability distribution is factorisable we are denying that the correlations between the individual properties are explained by the local factors incorporated in λ. In this way, denying this form of correlation amounts to saying that the correlations are inexplicable in terms of local variables.

This idea can be made more precise by considering two necessary conditions for factorisability to hold.

1. **Setting Independence:** $P(l|L, B, \lambda) = P(l|L, B', \lambda)$

   The outcome on the LHS does not depend on what measurement is performed on the RHS and vice versa.

2. **Outcome Independence:** $P(l|A, R, r, \lambda) = P(l, |A, R, r', \lambda)$

   The outcome of LHS does not depend on the outcome of the outcome of the RHS, except in so far as them both depend on λ.

These two conditions lead to factorisability as follows. Given outcome independence, it makes sense to talk of individual probability distributions for l and r, and so we can say that

$$P(l, r|L, R, \lambda) = P(l|L, R, \lambda)P(r|L, R, \lambda) \tag{2.24}$$

Given setting independence we can further say that

$$P(l|L, R, \lambda) = P(l|L, \lambda) \tag{2.25}$$

and similarly for r. It thus follows that

$$P(l, r|L, R, \lambda) = P(l|L, \lambda)P(r|R, \lambda) \tag{2.26}$$

which leads directly to the factorizability condition Eq. (2.23). Thus, if a system is not factorizable then either outcome independence or setting independence (or both) does not hold.

In addition to factorizability two further implicit, but seemingly very reasonable assumptions, are required.

1. "Single outcome assumption": On each run of the experiment only one result is obtained at each measuring device[6].

2. "No conspiracy assumption": On each run on the experiment we only obtain results for one of four possible measurements ($A\&B$, $A'\&B$, $A\&B'$, $A'\&B'$). We find the probabilities required to calculate C by averaging out over many runs of the experiment. We need to assume that bias is not introduced by the measuring technique so that the samples used to calculate the probabilities are fair.

[6] This may seem an odd assumption to explicitly state; however, it does not hold under the many worlds interpretation of quantum mechanics.

Once you have these two definitions the rest of the derivation is basic probability and algebra. In what follows we present the original derivation by Bell which is slightly more general than that presented in the psychic section. Specifically, we will aim to bound

$$C := |\langle LR\rangle - \langle LR'\rangle| + |\langle LR\rangle + \langle L'R\rangle| . \tag{2.27}$$

Using the factorisability condition we have

$$\langle LR\rangle = \sum_{l,r=\pm 1} lrP(l,r|L,R) \tag{2.28}$$

and similarly for the other terms in C.

Theorem 2.4.1. *Suppose that* ± 1 *are the only allowed values for* l *and* r*. The "outcome independence", "setting independence", "single outcome" and "no conspiracy assumptions" above imply that*

$$C \leq 2$$

for all choices of parameters l, r, l', r'*.*

Demo.

For convenience let us implicitly define

$$\langle LR\rangle := E_{L,R}(l\cdot r) := \int E_{L,R}(l\cdot r|\lambda)P(\lambda)d\lambda = \sum_{l,r=\pm 1} lrP(l,r|L,R)$$

where $E_{L,R}(l\cdot r)$ is the expectation value of the product $l\cdot r$ for a given choice of L and R. $E_{L,R}(l\cdot r|\lambda)$ represents the same quantity, conditioned on λ. Then we have

$$E_{L,R}(l,r|\lambda) = E_L(l|\lambda)E_R(r|\lambda) \quad \forall \lambda, L, R$$

from which

$$\begin{aligned} C &= |\langle LR\rangle - \langle LR'\rangle| + |\langle LR\rangle + \langle L'R\rangle| \\ &\leq \int \big[|E_L(l|\lambda)|\cdot|E_R(r|\lambda) - E_{R'}(r|\lambda)| + |E_R(r|\lambda)|\cdot|E_L(l|\lambda) + E_{L'}(l|\lambda)|\big]P(\lambda)d\lambda \\ &\leq \int \big[|E_R(r|\lambda) - E_{R'}(r|\lambda)| + |E_L(l|\lambda) + E_{L'}(l|\lambda)|\big]P(\lambda)d\lambda \end{aligned}$$

where the first inequality is taken from

$$\Big|\int f(x)dx\Big| \leq \int |f(x)|\, dx$$

and the second one

$$|E_\alpha(l|\lambda)| \leq 1$$

The proof of the theorem follows from

Lemme 2.4.2. *for* $x, y \in \mathbb{R}$ *and* $x, y \in [-1, 1]$ *we have* $|x-y| + |x+y| \leq 2$

Demo.

$$\begin{aligned} \big(|x-y| + |x+y|\big)^2 &= 2x^2 + 2y^2 + 2|x^2 - y^2| \\ &= \begin{cases} 4x^2 & x^2 > y^2 \\ 4y^2 & x^2 < y^2 \end{cases} \\ &\leq 4 \end{aligned}$$

□

Bell's non-locality theorem on its does not tell us which of setting and outcome independence is violated quantum mechanics. However, violation of either of those criterions is sufficient to show that quantum mechanics is in some sense non-local. Bell's non locality theorem tells us either that the setting of the other measuring device, or the particular measurement made, affects the measurement on the other electron.

Note that there is nothing to prevent the measurement events at the two different devices from being spacelike, and so in terms of our current physical theories causally, separated. As such, either the information concerning the setting of the other measuring device, or result of the other measurement, is communicated at greater than the speed of light. However the former would violate the no signalling theorem. Hence we conclude that Quantum Mechanics violates outcome independence not parameter independence.

The correlation coefficient is constructed to apply to any physical theory which makes predictions for the probability of results in any experimental set up of the general structure outlined above. In particular, the derivation makes no direct appeal to either quantum mechanics or determinism. Experiments have subsequently confirmed that the CHSH-Bell inequality is violated by our world. This tells us that any fundamental physical theory for the world we live in (not just quantum mechanics but also any theory that makes accurate predictions about our world!) must have non-local features.

2.5 Contextuality

The final quantum property we will discuss in this chapter is contextuality. It is a less discussed quantum property but nicely completes the set discussed in this chapter so we will cover it in brief. The best example to get a quick sense of contextuality is the Peres-Mermin (PM) square introduced by Kochen and Specker.

Here we consider a set of 9 different binary measurements we can perform each of which can give the outcomes ±1. Classically, we see this as being 9 properties of an object that we observe (+1) or do not observe (-1) in our system. We ask that observables in the same column or row form a context, or in other words, are jointly measurable.

$$\begin{bmatrix} A & B & C \\ a & b & c \\ \alpha & \beta & \gamma \end{bmatrix}$$

Let ABC denote the product of the values obtained from measuring A, B and C. Here, BC would be the measurement context of A. The observed properties can be probabilistic, so we define $\langle ABC \rangle = p(ABC = +1) - p(ABC = -1)$. We then consider (analogously to Bell inequalities) a correlation coefficient, this time of the form:

$$\langle PM \rangle = \langle ABC \rangle + \langle abc \rangle + \langle \alpha\beta\gamma \rangle + \langle Aa\alpha \rangle + \langle Bb\beta \rangle - \langle Cc\gamma \rangle \tag{2.29}$$

Classically we would expect measurements to be **noncontextual**. That is, we would expect the result of an observable to not depend on its context (the other measurements performed). If we assume our measurements are non-contextual then the maximum value the PM square can take is 4. In fact,

$$-4 \leq \langle PM \rangle \leq 4 \tag{2.30}$$

To see this note that the only way for the function f to have a value of 6 would be for all the products in the definition of f to be 1 except for the product cfi to be equal to -1. If the 5 first terms of the sum are all equals to 1, their product would also be equal to one, leading to:

$$a^2b^2d^2e^2g^2h^2cfi = 1,$$

implying that cfi is equal to 1. This proves that $f(M) \leq 4$. A similar argument can show that $f(M) \geq -4$.

However, by carefully picking our quantum observables, can show $\langle PM \rangle$ can *exceed* 4. For the table of quantum observables as follows

$$\begin{bmatrix} A & B & C \\ a & b & c \\ \alpha & \beta & \gamma \end{bmatrix} \quad \text{corresponding quantum example} \rightarrow \quad \begin{bmatrix} \sigma_z \otimes \mathbf{I} & \mathbf{I} \otimes \sigma_z & \sigma_z \otimes \sigma_z \\ \mathbf{I} \otimes \sigma_x & \sigma_x \otimes \mathbf{I} & \sigma_x \otimes \sigma_x \\ \sigma_z \otimes \sigma_x & \sigma_x \otimes \sigma_z & \sigma_y \otimes \sigma_y \end{bmatrix} \tag{2.31}$$

one can readily check that the columns and rows are made of commuting operators, and that the products of observables in the same contexts $\{A, B, C\}, ...$ are the identity except $Cc\gamma = -\mathbf{I}$. Thus we have $\langle PM \rangle = 6$ which violates Eq. (2.30). Note that this result is input state independent! Any two qubit state (entangled or unentangled) is contextual. It follows that quantum mechanics is **contextual**. Broadly contextuality can be understood as stemming from the fact that observables in quantum mechanics do not commute. (Like Bell's inequality, violations of the PM bound have been experimentally verified.)

Chapter 3

Identical multi-particle systems

In this section, we discuss the behaviour of identical quantum particles. We will explain how there are two sorts of identical particles distinguished by how their state changes when you swap two particle labels. At least initially in this section, we will switch back to working directly in terms of the wavefunction of particles because i. this is how this topic is conventionally taught, ii. it's good to stay fluent with both sets of notation and iii. I draw in part on Vincenzo Savona's notes here which were written in terms of wavefunctions. However, we could have equally phrased this section entirely in braket notation (or entirely in wavefunction notation).

3.1 Two identical particles

Consider a system with two particles labelled as 1 and 2. Suppose that each one-particle subsystem is described by wave functions $\phi_i(r_i)$ for $i \in \{1, 2\}$. How can you write the wavefunction of the joint system for 1 and 2? The most naive response, which would suggest that the product of one-particle wave functions satisfies the Schrödinger equation, fails in the general case. Indeed, such a solution, on the one hand, assumes that the probabilities of particle presence are entirely independent (which amounts, among other things, to neglecting all interactions between particles), and, on the other hand, potentially violates the linearity of the Schrödinger equation. More generally, for a system of two interacting particles through a potential $\hat{U}(\mathbf{r_1}, \mathbf{r_2})$, writing

$$\left(\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial \mathbf{r_1}^2} - \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial \mathbf{r_2}^2} + \hat{V}(\mathbf{r_1}) + \hat{V}(\mathbf{r_2}) + \hat{U}(\mathbf{r_1}, \mathbf{r_2})\right)\psi_1(\mathbf{r_1})\psi_2(\mathbf{r_2}) = E\psi_1(\mathbf{r_1})\psi_2(\mathbf{r_2},$$

presupposes that the two-particle Schrödinger equation:

$$\left(\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial \mathbf{r_1}^2} - \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial \mathbf{r_2}^2} + \hat{V}(\mathbf{r_1}) + \hat{V}(\mathbf{r_2}) + \hat{U}(\mathbf{r_1}, \mathbf{r_2})\right)\psi(\mathbf{r_1}, \mathbf{r_2}) = E\psi(\mathbf{r_1}, \mathbf{r_2}), \tag{3.1}$$

is separable, which is not necessarily true. We must find a way to describe the system using a single wave function that depends on all coordinates.

Suppose the particles are identical. This implies, among other things, that the probability $|\psi(\mathbf{r_1}, \mathbf{r_2})|^2$ of finding one particle at point $\mathbf{r_1}$ and the other at point $\mathbf{r_2}$ must be equal to $|\psi(\mathbf{r_2}, \mathbf{r_1})|^2$. In other words, we must have:

$$\psi(\mathbf{r_2}, \mathbf{r_1}) = e^{i\phi}\psi(\mathbf{r_1}, \mathbf{r_2})$$

Now this equation must hold for any $\mathbf{r_1}$ and $\mathbf{r_2}$ (if it did not it would imply that the space was non-isotropic[1]). This means it also holds in the case that $\mathbf{r_1} \to \mathbf{r_2}$ and $\mathbf{r_2} \to \mathbf{r_1}$ and so we also have

$$\psi(\mathbf{r_1}, \mathbf{r_2}) = e^{i\phi}\psi(\mathbf{r_2}, \mathbf{r_1})\,.$$

Combining these two equations then gives

$$\begin{aligned} &\psi(\mathbf{r_2}, \mathbf{r_1}) = e^{i2\phi}\psi(\mathbf{r_2}, \mathbf{r_1}) \\ \implies &e^{i2\phi} = 1 \\ \implies &e^{i\phi} = \pm 1. \end{aligned}$$

Now let's make this a bit more formal by defining $\mathbb{P}_{12}$ be the operator that acts on the system by interchanging particles 1 and 2. By the argument above, we know that for identical particles we have

$$\mathbb{P}_{1,2}\psi(\mathbf{r_1}, \mathbf{r_2}) = \psi(\mathbf{r_2}, \mathbf{r_1}) = \pm\psi(\mathbf{r_1}, \mathbf{r_2})\,.$$

Thus the permutation operator $\mathbb{P}_{1,2}$ has eigenvalues ± 1. We note that there is nothing[2] in the above argument that is unique to the vectors $\mathbf{r_1}$ and $\mathbf{r_2}$ being position vectors and so the argument equally applies to arbitrary vectors to the particle variables.

The eigenstates corresponding to the +1 eigenvalue are said to be symmetric under exchange (particles described by these functions are *bosons*) and the particles corresponding to the −1 operator are said to be antisymmetric under exchange (particles described by these functions are *fermions*). Fermions are half-integer spin particles such as electrons and quarks. Bosons are integer spin particles such as photons or gluons. This correlation with spin can be taken as an empirical fact in standard quantum mechanics.

Fermions. A direct consequence of the wavefunction of fermions being anti-symmetric under the particle permutation operator, i.e. $\mathbb{P}_{1,2}\psi(\mathbf{r_1}, \mathbf{r_2}) = \psi(\mathbf{r_2}, \mathbf{r_1}) = -\psi(\mathbf{r_1}, \mathbf{r_2})$, is that there is zero probability of finding two fermions in precisely the same state. More concretely, if $\psi(\mathbf{r}, \mathbf{r}) = -\psi(\mathbf{r}, \mathbf{r})$ then we must have that $\psi(\mathbf{r}, \mathbf{r}) = 0$.

Of course, a particle can possess more properties than a location. Let $|x\rangle = |m, \mathbf{r}, ...\rangle$ be a single quantum state to denote state dependent properties (e.g. its spin orientation m, position $\mathbf{r}$, ...) of a particle. We can then write a two particle state as

$$|\psi\rangle = \sum_{x,x'} a_{x,x'}\,|x, x'\rangle\;. \tag{3.2}$$

Note that now, rather than explicitly labelling the variables as corresponding to system 1 and 2 respectively as in $\psi(\mathbf{r_1}, \mathbf{r_2})$, I am taking the left and the right slots of the ket $|...\rangle|...\rangle$ to correspond to systems 1 and 2 respectively. In this formalism, for fermions we have

$$\mathbb{P}\,|x', x\rangle = |x, x'\rangle = -\,|x', x\rangle \tag{3.3}$$

[1]To see this, imagine $\mathbf{r_1}$ and $\mathbf{r_2}$ are single parameter variables and we place our coordinates such that the origin is midway between them. Now, we're considering $\psi(r, -r)$. Assuming the physics of the universe is invariant under reflections we are free to redefine $-r \leftrightarrow r$ without changing anything physical. Thus if $\psi(r, -r) = e^{i\phi}\psi(-r, r)$ we also have $\psi(-r, r) = e^{i\phi}\psi(r, -r)$. For arbitrary vectors we can also do the same trick of putting the coordinate system midway between the two particles and considering the axis that connects them.

[2]Ok this is where it gets super subtle. Technically my isotropy argument above did rely of these vectors being position vectors. However, for arbitrary variables, we can make an analogous argument saying that the action of the permutation operator should be independent of the variable it acts on. If this is getting too subtle do not worry about it- most discussion seems to gloss over these subtleties anyway.

Or, on the level of the full state, we can see that Eq. (3.3) implies that

$$\begin{aligned}\mathbb{P}|\psi\rangle &= \sum_{x,x'} a_{x,x'}\mathbb{P}|x,x'\rangle \\ &= \sum_{x,x'} -a_{x,x'}|x,x'\rangle = -|\psi\rangle.\end{aligned} \tag{3.4}$$

We now want to understand how the constraint $\mathbb{P}|\psi\rangle = -|\psi\rangle$ effects the allowed $a_{x,x'}$ values. To do this, note that

$$\begin{aligned}|\psi\rangle &= \sum_{x,x'} a_{x,x'}|x,x'\rangle \\ &= \sum_{x,x'} -a_{x,x'}|x',x\rangle \\ &= \sum_{x,x'} -a_{x',x}|x,x'\rangle\end{aligned} \tag{3.5}$$

where in the first line we use Eq. 3.3 and in the second (as we are summing over both x and x') we are free to perform the relabelling $x \to x'$ and $x' \to x$. Thus comparing the first and final line of Eq. (3.5) we see that

$$a_{x,x'} = -a_{x',x} \tag{3.6}$$

and

$$a_{x,x} = 0\,. \tag{3.7}$$

This is the core of what is known as the ***Pauli exclusion principle*** - no two fermions can occupy the same single particle quantum state. Note that while no two fermions with the same spin can occupy the same position, if the fermions spin differ then there can be a non-zero amplitude of finding the two fermions at the same position. That is, electrons in different spin states can be in the same place but electrons in the same spin state avoid one another[3].

Any expansion of a two-fermion state, i.e., Eq. (3.2), involves an even number of terms because from Eq. (3.6) any term of the form $a_{x,x'}$ comes with its negative swapped partner $-a_{x',x}$. The simplest such state of this form corresponds to the case where each electron can take one of two different spin states. Let us label these $|0\rangle$ and $|1\rangle$ and so as $a_{0,1} = -a_{1,0}$ and $a_{0,0} = a_{1,1} = 0$, we obtain

$$|\psi\rangle \propto |0,1\rangle - |1,0\rangle \quad \to \quad |\psi\rangle = \frac{1}{\sqrt{2}}\left(|0,1\rangle - |1,0\rangle\right) := |\Psi_-\rangle\,. \tag{3.8}$$

Thus we see that the simplest possible two particle fermionic state is the singlet Bell state $|\Psi_-\rangle$. To check that this works we note that:

$$\mathbb{P}|\psi\rangle = \frac{1}{\sqrt{2}}\left(\mathbb{P}|0,1\rangle - \mathbb{P}|1,0\rangle\right) = \frac{1}{\sqrt{2}}\left(|1,0\rangle - |0,1\rangle\right) = -\frac{1}{\sqrt{2}}\left(|0,1\rangle - |1,0\rangle\right) = -|\psi\rangle\,. \tag{3.9}$$

Boson. Let us now see what happens if we repeat the same calculation above but suppose the identical particles are bosons. This time we have $\mathbb{P}|x,x'\rangle = |x',x\rangle = |x,x'\rangle$, and so we can write

$$|\psi\rangle = \sum_{x,x'} a_{x,x'}|x,x'\rangle = \sum_{x,x'} a_{x,x'}|x',x\rangle = \sum_{x,x'} a_{x',x}|x,x'\rangle\,, \tag{3.10}$$

where in the second equality we relabel $x \to x'$ and $x' \to x$. It follows that

$$a_{x,x'} = a_{x',x}\,. \tag{3.11}$$

[3] There is a cliched comparison you could make here between electrons and fashionable folk accidentally in the same outfit at a party not wanting to be seen together.

This time we can have non-zero amplitudes for both particles to be in the same state, i.e., have $a_{x,x} \neq 0$. But any amplitude of the form $a_{x,x'}$ comes with an identical amplitude of the form $a_{x',x}$. Consider two photons that can be in the states $|0\rangle$ or $|1\rangle$, the allowed basic states are

$$|0,0\rangle\,, |1,1\rangle\,, \frac{1}{\sqrt{2}}\left(|0,1\rangle + |1,0\rangle\right)\,. \tag{3.12}$$

$$\tag{3.13}$$

We can then of course also consider superpositions of these states, eg. $\cos(\theta)\,|0,0\rangle + e^{i\phi}\sin(\theta)\,|1,1\rangle$.

3.2 Multiple identical particles

This reasoning generalizes to systems of n particles, where $n \in \mathbb{N}$. Let $\psi(\mathbf{r_1}, \cdots, \mathbf{r_n})$ be the wave function of the system. First of all, note that exchanging particle j and particle k for $j,\ k \in \{1, \cdots, n\}$ is equivalent to exchanging particle k and particle j, i.e., $\mathbb{P}_{j,k} = \mathbb{P}_{k,j}$. Furthermore,

$$\begin{aligned}
\mathbb{P}_{j,k}\left(\mathbb{P}_{j,k}\psi(\mathbf{r_1}, \cdots, \mathbf{r_j}, \cdots, \mathbf{r_k}, \cdots, \mathbf{r_n})\right) &= \mathbb{P}_{j,k}\left(\psi(\mathbf{r_1}, \cdots, \mathbf{r_j}, \cdots, \mathbf{r_k}, \cdots, \mathbf{r_n})\right) \\
&= \psi(\mathbf{r_1}, \cdots, \mathbf{r_j}, \cdots, \mathbf{r_k}, \cdots, \mathbf{r_n}) \\
&= \mathbb{1}\left(\psi(\mathbf{r_1}, \cdots, \mathbf{r_j}, \cdots, \mathbf{r_k}, \cdots, \mathbf{r_n})\right),
\end{aligned}$$

so, $\mathbb{P}_{j,k}\mathbb{P}_{j,k} = \mathbb{1}$, and $\mathbb{P}_{j,k}^{-1} = \mathbb{P}_{j,k} = \mathbb{P}_{k,j}$. Finally, the sign of the operator $\mathbb{P}_{j,k}$ must be the same for all $j,\ k \in \{1, \cdots, n\}$. In fact:

$$\mathbb{P}_{j,k} = \mathbb{P}_{1,j}\mathbb{P}_{2,k}\mathbb{P}_{1,2}\mathbb{P}_{2,k}\mathbb{P}_{1,j}.$$

A "permutation operator" is an operator of the form $\mathbb{P} = \prod \mathbb{P}_{j,k}$. It follows that wavefunctions corresponding to eigenvalues of a permutation operator are either symmetric or antisymmetric. This is the *symmetry postulate*, which can be restated as follows:

Symmetrisation Postulate (Cohen-Tannoudji, Diu, Laloe, 1977**)** : When a state includes several identical particles, only certain kets of its state space can describe its physical state. Physical kets are, depending on the nature of its identical particles, either completely symmetric or completely anti-symmetric with respect to the permutation of these particles. Those particles for which the physical kets are symmetric are called bosons, and those for which they are antisymmetric, fermions.

Notice that this has important consequences in the description of the physics of the system. Consider, for example, an arbitrary observable $\hat{O}$ of the system. Using the above, its average value must satisfy, for all $j,\, k \in \mathbb{N}$:

$$\langle\psi|\hat{O}|\psi\rangle = \langle\psi|\mathbb{P}_{j,k}^{\dagger}\hat{O}\mathbb{P}_{j,k}|\psi\rangle\,,$$

which implies $\hat{O} = \mathbb{P}_{j,k}^{\dagger}\hat{O}\mathbb{P}_{j,k}$, and the operator $\mathbb{P}_{j,k}$ commutes with all observables. In particular, if $\hat{H}$ is the system's Hamiltonian, $[\mathbb{P}_{jk}, \hat{H}] = [\hat{H}, \mathbb{P}_{jk}]$ for all $j,\, k \in \mathbb{N}$. Physically, this result is expected: Since the particles are assumed to be identical, there is no reason for the system's Hamiltonian to be modified by the exchange of two particles. As per what was previously discussed, since all $\mathbb{P}_{j,k}$ have the same sign, we can always simultaneously diagonalize $\mathbb{P}$ and $\hat{H}$. In other words, $[\mathbb{P}, \hat{H}] = 0$ for any operator $\mathbb{P}$.

3.2.1 Bosons

Let's now consider the possible basis states for a system of n Bosons. For two Bosons these were:

$$|00\rangle,\ |11\rangle,\ \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle)\,. \tag{3.14}$$

This can equivalently be written as

$$|\psi_{\mathbf{x}}\rangle \propto \sum_{\mathbb{P}\in S_2} \mathbb{P}|x_1, x_2\rangle = \sum_{\mathbb{P}\in S_2} |\mathbf{x}_{\mathbb{P}(1)}\rangle|\mathbf{x}_{\mathbb{P}(2)}\rangle \tag{3.15}$$

where $\mathbf{x} = (x_1, x_2)$ and S_n is the symmetric group on n elements. We will formally define S_n later in term, for now just think of it as the set of all possible permutations of n objects. When $n = 2$ this is just the identity operation and the swap operation. For example, for the case of $x_1 = 0$, $x_2 = 0$ we have

$$|\psi_{\mathbf{x}}\rangle \propto \sum_{\mathbb{P}\in S_2} \mathbb{P}|00\rangle = \mathbb{I}|00\rangle + \mathbb{P}_{12}|00\rangle = |00\rangle + |00\rangle = 2|00\rangle \xrightarrow{\text{normalization}} |00\rangle \tag{3.16}$$

where as for $x_1 = 0$, $x_2 = 1$ we have

$$|\psi_{\mathbf{x}}\rangle \propto \sum_{\mathbb{P}\in S_2} \mathbb{P}|01\rangle = \mathbb{I}|01\rangle + \mathbb{P}_{12}|01\rangle = |01\rangle + |10\rangle \xrightarrow{\text{normalization}} \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle)\,. \tag{3.17}$$

Thus we see that Eq. (3.21) gives the correct expression for the basis states up to normalization. This expression generalizes to an n particles system as you would expect:

$$|\psi_{\mathbf{x}}\rangle = \mathcal{N}\sum_{\mathbb{P}\in S_n} \mathbb{P}|x_1, x_2, \ldots, , x_n\rangle \propto \sum_{\mathbb{P}\in S_n} \mathbb{P}|x_1, x_2, \ldots, , x_n\rangle = \sum_{\mathbb{P}\in S_n} |\mathbf{x}_{\mathbb{P}(1)}\rangle|\mathbf{x}_{\mathbb{P}(2)}\rangle\ldots|\mathbf{x}_{\mathbb{P}(n)}\rangle\,. \tag{3.18}$$

where $\mathcal{N}$ is a normalization factor. For example, if we consider a three particle system and $x_1 = 0$, $x_2 = 1$, $x_3 = 2$, as expected we obtain

$$\begin{aligned}|\psi_{\mathbf{x}}\rangle \propto \sum_{\mathbb{P}\in S_2} \mathbb{P}|001\rangle &= \mathbb{I}|001\rangle + \mathbb{P}_{12}|001\rangle + \mathbb{P}_{13}|001\rangle + \mathbb{P}_{23}|001\rangle + \mathbb{P}_{123}|001\rangle + \mathbb{P}_{132}|001\rangle \\ &= |001\rangle + |001\rangle + |100\rangle + |010\rangle + |100\rangle + |010\rangle \\ &= |001\rangle + |010\rangle + |001\rangle \\ &\xrightarrow{\text{normalization}} \frac{1}{\sqrt{3}}(|001\rangle + |010\rangle + |001\rangle)\,.\end{aligned} \tag{3.19}$$

What about the normalization factor $\mathcal{N}$? Well, there are $n!$ ways of permuting n objects. If the vector $\mathbf{x}$ contains no repeated entries then each of the corresponding states resulting from the permutation are unique and the normalization is simply $\frac{1}{\sqrt{n!}}$. If there are repeated entries however (e.g. as we saw in Eq.(3.16)) normalization you get an extra factor in the numerator that needs to be accounted for. Specifically, if you have n_k repeated entries you have $n_k!$ identical terms in the sum. Hence the normalization factor is

$$\mathcal{N} = \frac{1}{\sqrt{n!}\sqrt{\prod_k n_k!}} \tag{3.20}$$

where $\sum_k n_k = n$. *Exercise: Derive Eq.* (3.20) *for yourself more carefully.*

3.2.2 Fermions

It is also possible to write a general expression for the basis states of a Fermion. In analogy with Eq. (3.18) above, one has

$$|\psi_{\mathbf{x}}\rangle = \frac{1}{\sqrt{n!}} \sum_{\mathbb{P}\in S_n} \operatorname{sign}(\mathbb{P})\mathbb{P}|x_1, x_2, \ldots, , x_n\rangle \,. \tag{3.21}$$

where $\operatorname{sign}(\mathbb{P}) = -1$ if $\mathbb{P}$ involves an odd number of index swaps and $\operatorname{sign}(\mathbb{P}) = 1$ if $\mathbb{P}$ involves an even number of index swaps. We note that given the Pauli exclusion principle, no two Fermions can be in the same state (i.e. $n_k = 1$ for all k), so each state in the sum here is unique and so the normalization is simply $\frac{1}{\sqrt{n!}}$.

3.3 Distinguishing identical particles

At this point, it is perhaps valuable to take a step back and think about how the symmetrisation postulate fits with our understanding of the physics of quantum particles / the world around us more generally.

As the universe is a system containing large numbers of identical particles, the symmetrisation postulate tells us that all identical particles in the universe are in a state with particles of the same type that is symmetric or anti-symmetric under exchange. Either way, as the global phase in quantum mechanics does not correspond to anything physical, this entails that all identical particles of the same type are in a (typically highly entangled!) permutation invariant state. It follows that all identical particles, understood as represented by the indices in the quantum state, share with other particles of the same type both their intrinsic properties and state dependent properties[4].

However, this description of fundamental particles is far from our usual treatment of identical particles. An electron is a fermion but we do not usually think of electrons as being permutable and in exactly the same state as every other particle in the universe. Rather electrons are charge carriers in wires, they are in the shells of atoms, they exist in plasmas and so forth. We take electrons to exist wholly within reasonably well defined finite systems.

In practice, we are able to talk about electrons in such reasonably well defined localised roles by identifying stable dynamical properties. These stable dynamical properties enable us to distinguish subsystems of the total symmetrised state of fermions. These stable dynamical properties will typically be spatial. However, they need not be.

Consider a state of two identical particles in the orthogonal states $|\phi\rangle$ and $|\psi\rangle$. The state of the system can be described by:

$$|\Psi\rangle = \frac{1}{\sqrt{2}}[1 + \epsilon\mathbb{P}_{12}]\,|\phi, \psi\rangle \tag{3.22}$$

where $\epsilon = 1$ for bosons and $\epsilon = -1$ for fermions.

Say we are interested in the observable $\hat{Q}$ where $\hat{Q}\,|u_i\rangle = q_i\,|u_i\rangle$. Using the Born rule, the probability amplitude, of obtaining q_i and q_j on measurement, is:

$$\begin{aligned} &1/2\,\langle u_i, u_j|\,[1 + \epsilon\mathbb{P}_{21}^{\dagger}][1 + \epsilon\mathbb{P}_{21}]\,|\phi, \psi\rangle \\ &= \langle u_i\phi\rangle\langle u_j\psi\rangle + \epsilon\langle u_i\psi\rangle\langle u_j\phi\rangle \,. \end{aligned}$$

[4]If you are looking over these notes having already read Chapter 3, identical particles have the same 'state dependent properties' in the sense that they all have the same reduced density operator (obtained by taking the partial trace).

The first term is known as the direct integral and the second is the exchange integral.

The state of a pair of non-identical (i.e. non-permutable) particles in the orthogonal states $|\phi\rangle$ and $|\psi\rangle$ respectively is written $|\psi\rangle \otimes |\phi\rangle$. In this case, the probability of measuring q_i, q_j is simply $|\langle u_i \psi\rangle\langle u_j \phi\rangle|^2$.

This suggests the following operational claim: Particle permutation between a pair of particles can be ignored when either the direct or exchange integral between that pair of particles vanishes. Otherwise, the symmetry postulate entails that permutation must be taken into account.

One way in which one of the integrals can disappear is if both the particles and the measuring devices are spatially separated. Say, the wavepackets of the identical particles are well localised and spatially separated such that $\langle x|\psi\rangle = 0$ if x is in the region R and $\langle x|\phi\rangle = 0$ if x is in the region L. Similarly, suppose the measuring device wavepackets are spatially separated such that $\langle x|u_i\rangle = 0$ if x is in the region R and $\langle x|u_j\rangle = 0$ if x is in the region of L. Thus we have

$$\langle u_j|\psi\rangle = \sum_x \langle u_j|x\rangle\langle x|\psi\rangle = 0 \tag{3.23}$$

and as such the exchange integral disappears[5]. When this is the case we can identify each particle by its well defined positions and we say things like 'the particle on the left is in state ψ' and 'the particle on the right is in state ϕ' and write $|\psi, \phi\rangle$ where the left and right slots correspond to the left and right electrons respectively.

We make use of the vanishing exchange integral between pairs of spatially separated systems and measuring devices when we wish to consider a particular subset of particles in the universe. We can consider a pair of electrons in a shell of helium and treat these two electrons as permutable, without needing to consider permutations between these two electrons and all other electrons in the universe. It is also the reason why, combined with the fact that the position and spin operators commute, we do not have to take into account the symmetric spatial part of the wavefunction in Bell type experimental setups.

However, there is nothing fundamentally special about position. We could equally have used a different stable dynamical property to distinguish the particles. For example, if spin dependent interactions are negligible in a scattering experiment then the different spin alignments of a pair of particles can be used to treat the two particles that scatter as non-permutable. Consider the following initial state for the collision problem sketched in Fig. 3.1,

$$|\Psi_{\text{initial}}\rangle = \frac{1}{\sqrt{2}}\left[1 + \epsilon\mathbb{P}_{12}\right]|p_{\mathbf{z}}, +, -p_{\mathbf{z}}, -\rangle\ . \tag{3.24}$$

Here $|p_{\mathbf{z}}, +\rangle$ denotes the state of the particle with momentum in the positive z direction and spin z of $+\frac{1}{2}$ (and conversely for $|-p_{\mathbf{z}}, -\rangle$). Say we are interested in knowing the probability that the system is in the final state

$$|\Psi_{\text{final}}\rangle = \frac{1}{\sqrt{2}}\left[1 + \epsilon\mathbb{P}_{12}\right]|p_{\mathbf{v}}, +, -p_{\mathbf{v}}, -\rangle \tag{3.25}$$

where $\pm p_{\mathbf{v}}$ denotes momentum in the plus and minus $\mathbf{v}$ directions sketched in Fig. 3.1b).

The evolution operator responsible for the collision, $\hat{U}(t, t_0)$, commutes with the permutation operator. Thus we have

$$\hat{U}(t,t_0)\,|\Psi_{\text{initial}}\rangle = \frac{1}{\sqrt{2}}(\hat{U}(t,t_0)\,|p_{\mathbf{z}}, +, -p_{\mathbf{z}}, -\rangle + \epsilon\hat{U}(t,t_0)\,|-p_{\mathbf{z}}, -, p_{\mathbf{z}}, +\rangle \tag{3.26}$$

[5]There is nothing significant about the exchange rather than direct integral disappearing. I could have swapped the location of the measurement devices for the converse.

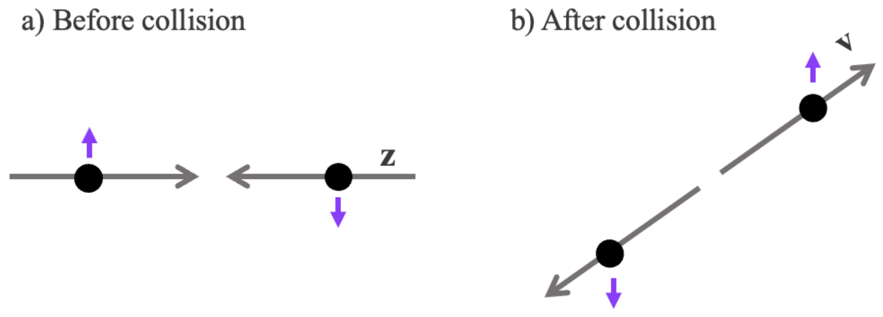


Figure 3.1: Diagram of a collision experiment with no spin interaction ((Cohen-Tannoudji, Diu, Laloe, 1977).)

and so

$$\langle \Psi_{\text{final}}| \hat{U}(t,t_0) |\Psi_{\text{initial}}\rangle \propto \langle p_{\mathbf{v}}, +, -p_{\mathbf{v}}, -| \hat{U}(t,t_0) |p_{\mathbf{z}}, +, -p_{\mathbf{z}}, -\rangle + \epsilon \langle p_{\mathbf{v}}+, -p_{\mathbf{v}}-| \hat{U}(t,t_0) |-p_{\mathbf{z}}, -, p_{\mathbf{z}}, +\rangle \tag{3.27}$$

Now we are interested in the case where $\hat{U}(t,t_0)$ does not affect spin interactions. As such, the exchange term is sandwiched between two orthogonal states and vanishes, and so we are left with

$$\langle \Psi_{\text{final}}| \hat{U}(t,t_0) |\Psi_{\text{initial}}\rangle \propto \langle p_{\mathbf{v}}, +, -p_{\mathbf{v}}, -| \hat{U}(t,t_0) |p_{\mathbf{z}}, +, -p_{\mathbf{z}}, -\rangle \,. \tag{3.28}$$

That is, we are left with the probability associated with two non-permutable particles.

In both the case of the spatially separated particles and the particle denoted by its spin, operationally we are free to work directly with states labelled according to their distinguishing properties:

$$\frac{1}{\sqrt{2}}(1+\epsilon\mathbb{P}_{12})\,|\phi,\psi\rangle \to |\phi\rangle_L \otimes |\psi\rangle_R \tag{3.29}$$

$$\frac{1}{\sqrt{2}}(1+\epsilon\mathbb{P}_{12})\,|p_{\mathbf{z}}, +, -p_{\mathbf{z}}, -\rangle \to |p_{\mathbf{z}}\rangle_+ |-p_{\mathbf{z}}\rangle_- \tag{3.30}$$

What do we conclude from these examples? The symmeterisation postulate is a fundamental theorem in quantum mechanics that implies that all identical fermions are in an anti-symmetric entangled state. However, this does not mean that we need to consider this state in practise most of the time. If there are stable dynamical properties to distinguish quantum two electrons over time, we can label those electrons by those properties and just those two properties (i.e. the electron on the left/the electron on the right or the spin up electron/spin down electron). In practise, this treatment of permutable particles is empirically successful and what we end up working with most of the time.

3.4 Second Quantization:

Second quantization is an approach used to represent systems composed of multiple particles. We consider a situation where the number of particles can potentially change, noting that a particle's state is entirely determined by the one-particle functions in the basis of $\mathcal{H}_1$. We construct the *Fock space* where kets indicate the number of times a wave function is involved.

For example, the transformation from 1st quantisation (what we have been discussing so far in this chapter) to second quantisation looks like

$$\begin{aligned} &\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) \to |11\rangle \\ &|\uparrow\uparrow\rangle \to |20\rangle \\ &|\downarrow\downarrow\rangle \to |02\rangle\,. \end{aligned} \tag{3.31}$$

Here the left and right slots in the Fock basis indicate the number of Bosons in the $\uparrow$ and $\downarrow$ states respectively. Similarly, for Fermions we could have

$$\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) \to |11\rangle\,. \tag{3.32}$$

It's worth noting that for bosons, the n_i appearing in $|n_1, n_2, \cdots\rangle$ can be arbitrary, while for fermions, they can only take the values 0 or 1 due to the Pauli exclusion principle. Also note that it's important once in the second quantisation to know whether the state you are looking at is a Fermionic of Bosonic state as, for example, a state of the form $|11\rangle$ could refer to either but behaves differently in the two cases.

We introduce creation and annihilation operators to increase or decrease the number of particles.

- The Bosonic case is entirely analogous with the case of a simple harmonic oscillator which you should be familiar with from Quantum Physics 1. Specifically we have:

$$\begin{cases} \hat{c}_i^\dagger\,|n_1, \cdots, n_i, \cdots\rangle = \sqrt{n_i + 1}\,|n_1, \cdots, n_i + 1, \cdots\rangle\,, \\ \hat{c}_i\,|n_1, \cdots, n_i, \cdots\rangle = \sqrt{n_i}\,|n_1, \cdots, n_i - 1, \cdots\rangle\,, \end{cases}$$

  It follows that (*check this!*) that creation and annihilation operators in the bosonic case satisfy:

  - $[\hat{c}_i, \hat{c}_j] = [\hat{c}_i^\dagger, \hat{c}_j^\dagger] = 0$
  - $[\hat{c}_i, \hat{c}_j^\dagger] = \delta_{ij}$.

- The Fermionic case is much more subtle. In this case we need to ensure that the resulting states are antisymmetric under exchange. This can be achieved by defining the creation and annihilation operators as follows:

$$\begin{cases} \hat{c}_i^\dagger\,|n_1, \cdots, n_i, \cdots\rangle = (-1)^{n_1 + \cdots + n_{i-1}}(1 - n_i)\,|n_1, \cdots, n_i + 1, \cdots\rangle\,, \\ \hat{c}_i\,|n_1, \cdots, n_i, \cdots\rangle = (-1)^{n_1 + \cdots + n_{i-1}} n_i\,|n_1, \cdots, n_i - 1, \cdots\rangle\,, \end{cases}$$

  To get a sense of the form of these expressions first notice that the $(1 - n_i)$ factor ensures that you cannot create Fermionic states with more than one particle in the same state.

  The factor of $(-1)^{n_1 + \cdots + n_{i-1}}$ then ensures the antisymmetrisation. For example, we require that $\hat{c}_0^\dagger \hat{c}_1^\dagger|00\rangle = -\hat{c}_1^\dagger \hat{c}_0^\dagger|00\rangle$. We indeed have this as $\hat{c}_0^\dagger \hat{c}_1^\dagger|00\rangle = \hat{c}_0^\dagger(-1)^0|01\rangle = |11\rangle$ and $\hat{c}_1^\dagger \hat{c}_0^\dagger|00\rangle = \hat{c}_1^\dagger|10\rangle = (-1)^1|11\rangle = -|11\rangle$. The general case can be understood by iterating this argument.

  It is straightforward to verify (*check this!*) that the creation and annihilation operators in the fermionic case satisfy:

  - $\{\hat{c}_i, \hat{c}_j\} = \{\hat{c}_i^\dagger, \hat{c}_j^\dagger\} = 0$
  - $\{\hat{c}_i, \hat{c}_j^\dagger\} = \delta_{ij}$

  where $\{A, B\} = AB + BA$.

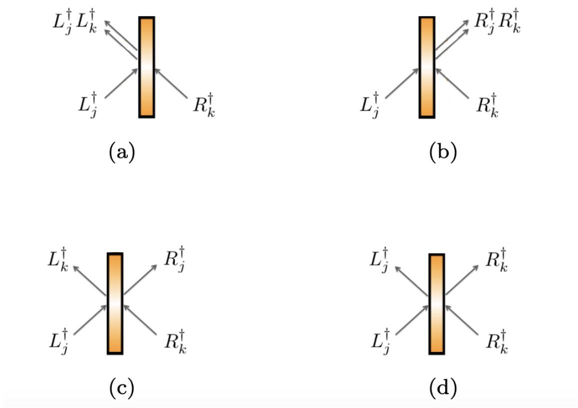


Figure 3.2: The Hong-Ou-Mandel effect and Bosonic bunching.

3.5 The Hong-Ou-Mandel Effect and Bosonic Bunching

To get a bit of practise of working in the second quantisation, and as another illustration of the difference between fermions and bosons, we'll end this chapter by presenting something called the Hong-Ou-Mandel (HOM) effect. The HOM effect describes what happens when two identical photons hit a beamsplitter. It shows that while fermions have a tendency to avoid each other, bosons have a tendency to clump together.

When working in the second quantisation it is often helpful to work in the Heisenberg picture and consider the action of any unitary process on the creation and annihilation operators rather than on a given state directly. Suppose we have a photon impinge on a 50-50 beamsplitter as shown in Fig. 3.3. Let $\hat{L}_H$, $\hat{L}_V$, $\hat{R}_H$, $\hat{R}_V$ denote the annihilation operators for horizontally and vertically polarised photons on the left and right hand side of the beamsplitter. The action of this beamsplitter can be modelled in the Heisenberg picture as

$$\begin{aligned} \hat{L}_k^\dagger &\to \frac{1}{\sqrt{2}}(\hat{L}_k^\dagger + \hat{R}_k^\dagger) \\ \hat{R}_k^\dagger &\to \frac{1}{\sqrt{2}}(\hat{L}_k^\dagger - \hat{R}_k^\dagger) \end{aligned} \tag{3.33}$$

for $k = H$ and $k = V$ and where the minus sign in the second line above is to ensure unitarity.

When an H photon and a V photon (i.e. two perfectly distinguishable photons) impinge on opposite sides of a beamsplitter simultaneously we have

$$\begin{aligned} |1\rangle_{LH}|0\rangle_{LV}|0\rangle_{RH}|1\rangle_{RV} = \hat{L}_H^\dagger \hat{R}_V^\dagger|0000\rangle \to\ & \frac{1}{2}(\hat{L}_H^\dagger + \hat{R}_H^\dagger)(\hat{L}_V^\dagger - \hat{R}_V^\dagger)|0000\rangle \\ =\ & \frac{1}{2}(-|1\rangle_{LH}|0\rangle_{LV}|0\rangle_{RH}|1\rangle_{RV} + |1\rangle_{LH}|1\rangle_{LV}|0\rangle_{RH}|0\rangle_{RV} \\ & - |0\rangle_{LH}|0\rangle_{LV}|1\rangle_{RH}|1\rangle_{RV} + |0\rangle_{LH}|1\rangle_{LV}|1\rangle_{RH}|0\rangle_{RV}) \end{aligned} \tag{3.34}$$

That is, there are four equally probable outcomes as sketched in Fig. 3.3:

(a) the photon from the right is transmitted and the photon from the left is reflected,

(b) the photon from the left is transmitted and the photon from the right is reflected,

(c) both photons are transmitted,

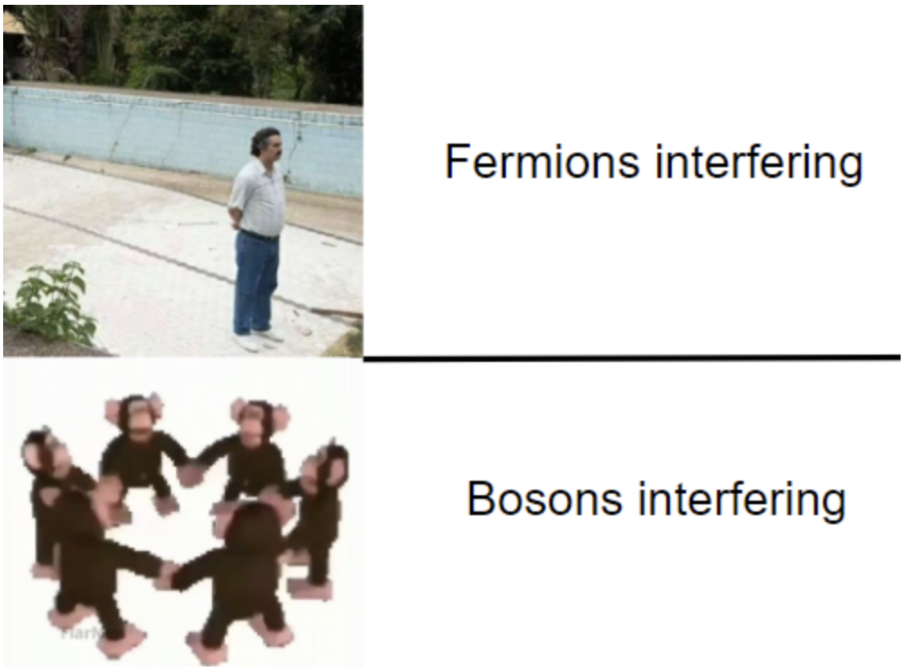


Figure 3.3: Credit: Nicolas Emile Bourquin

(d) both photons are reflected.

However, when the two photons are indistinguishable, something intriguing happens. Suppose both photons are horizontally polarized (and the same frequency etc). In this case (dropping the unchanged vacuum V modes for simplicity) we have

$$\begin{aligned} |1\rangle_{LH}|1\rangle_{RH} = \hat{L}_H^\dagger \hat{R}_H^\dagger |00\rangle &\to \frac{1}{2}(\hat{L}_H^\dagger + \hat{R}_H^\dagger)(\hat{L}_H^\dagger - \hat{R}_H^\dagger)|00\rangle \\ &= \frac{1}{2}\left(\hat{L}_H^{\dagger\,2} - \hat{R}_H^{\dagger\,2}\right)|00\rangle \\ &= \frac{1}{\sqrt{2}}(|2\rangle_{LH}|0\rangle_{RH} - |0\rangle_{LH}|2\rangle_{RH}) \end{aligned} \tag{3.35}$$

The amplitude for both photons to be reflected by the BS and the amplitude for both photons to be transmitted through the BS have destructively interfered, and thus the probability for the photons to exit the beamsplitter through opposite sides vanishes. Indistinguishable photons are therefore guaranteed to leave a beamsplitter in the same mode, a phenomenon known as 'bosonic bunching'.

Chapter 4

Reduced and mixed quantum states

So far we have represented quantum states as a vector $|\psi\rangle$. Density operators, whereby a quantum state is represented by a matrix ρ, is an alternative formalism for representing quantum states. In particular, this perspective will allow us to- i. handle classical uncertainty as well as quantum uncertainty in a single formalism and ii. extract the state of part of a quantum system from knowledge of its composite system.

4.1 Density operators

The *density operator* corresponding to a state $|\psi\rangle$ is given by the matrix $\rho = |\psi\rangle\langle\psi|$. The average value of an observable $\hat{O}$ in the state ρ is then given by:

$$\left\langle \hat{O} \right\rangle = \mathrm{Tr}(|\psi\rangle\langle\psi|\hat{O}) \tag{4.1}$$

To see that this does indeed give same expectation value as the standard state vector formalism just apply the cyclicity of the trace directly to Eq. (4.1).

Examples 4.1.1.

1. The state $|\psi\rangle = |1\rangle$ is a pure state of the system, and the corresponding density operator ρ is given by:

$$\rho = |\psi\rangle\langle\psi| = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}.$$

2. The state $|+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ is written in density matrix form as:

$$\rho = \begin{pmatrix} \frac{1}{2} & \pm\frac{1}{2} \\ \pm\frac{1}{2} & \frac{1}{2} \end{pmatrix}.$$

3. <u>Bell States:</u> The density operator corresponding to the Bell state $|\Psi_-\rangle = \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle)$ is given by:

$$\rho = \frac{1}{2}\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$

Density operators open up a new perspective on the Bloch sphere. To see this first note that density operator of a single qubit $\cos(\theta/2)|0\rangle + e^{i\phi}\sin(\theta/2)|1\rangle$ can be written as

$$\rho = |\psi\rangle\langle\psi| = \begin{pmatrix} \cos(\theta/2)^2 & \cos(\theta/2)\sin(\theta/2)e^{-i\phi} \\ \cos(\theta/2)\sin(\theta/2)e^{i\phi} & \sin(\theta/2)^2 \end{pmatrix} \tag{4.2}$$

Next we note that any 2×2 matrix can be written as a weighted sum of the Pauli matrices,

$$\{\sigma_i\}_{i=0}^3 := \{\mathbb{1}, \sigma_x, \sigma_y, \sigma_z\} = \left\{ \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right\} \tag{4.3}$$

because Pauli matrices form an orthogonal basis with the following helpful properties

$$\mathrm{Tr}[\sigma_0] = 1, \mathrm{Tr}[\sigma_k] = 0 \ \text{ for } \ k \neq 0 \tag{4.4}$$
$$\mathrm{Tr}[\sigma_j \sigma_k] = 2\delta_{k,j} \ . \tag{4.5}$$

It follows that we can write

$$\rho = \frac{1}{2}\sigma_0 + \frac{1}{2}\sum_{i=1}^{3} v_i \sigma_i \tag{4.6}$$

where the factor of 2 is to account for the factor of 2 in $\mathrm{Tr}[\sigma_j \sigma_k] = 2\delta_{k,j}$.

Next we ask, what is the significance of the vector $\mathbf{v} = (v_1, v_2, v_3)$ in Eq. (4.6). To answer this - we first note that it follows from the properties of the Pauli matrices (namely, $\mathrm{Tr}[\sigma_j \sigma_k] = 2\delta_{k,j}$) that $v_i = \mathrm{Tr}[\rho \sigma_i]$. It follows that the vector $\mathbf{v}$ is a vector of the expectation values of the Pauli observables:

$$\mathbf{v} = \begin{pmatrix} \langle \sigma_x \rangle \\ \langle \sigma_y \rangle \\ \langle \sigma_z \rangle \end{pmatrix} . \tag{4.7}$$

Alternatively, we one can verify by direct comparison of Eq. (4.2) and Eq. (4.6) (check this for yourself!) that

$$\mathbf{v} = \begin{pmatrix} \sin(\theta)\cos(\phi) \\ \sin(\theta)\sin(\phi) \\ \cos(\theta) \end{pmatrix} . \tag{4.8}$$

That is, the vector $\mathbf{v}$ is the unit Bloch vector which can be used to represent a quantum state on the Bloch sphere.

Thus far this switch in representation may seem rather arbitrary. We have provided a different perspective on quantum states but not done anything more. The real power of this formalism will be made clearer in the following two sections.

4.1.1 Pure states and mixed states

Suppose someone prepares a system S in the state $|\psi\rangle$ with probability p and state $|\phi\rangle$ with probability $1 - p$ by tossing a biased coin, how would we mathematically represent the state of the system S? We we want a mathematical entity that allows us to correctly compute the expectation value of any observable $\hat{O}$. Now we know from basic probability that the expectation of $\hat{O}$ should be

$$\begin{aligned} \langle \hat{O} \rangle &= p\langle \hat{O} \rangle_\psi + (1-p)\langle O \rangle_\phi \\ &= p \langle \psi | \hat{O} | \psi \rangle + (1-p) \langle \phi | \hat{O} | \phi \rangle \\ &= p\,\mathrm{Tr}(|\psi\rangle\langle\psi|\hat{O}) + (1-p)\,\mathrm{Tr}(|\phi\rangle\langle\phi|\hat{O}) \\ &:= \mathrm{Tr}(\rho\hat{O}) \end{aligned}$$

where we have used $\mathrm{Tr}(|\psi\rangle\langle\psi|\hat{O}) = \langle\psi| \hat{O} |\psi\rangle$ and in the final line defined

$$\rho := p|\psi\rangle\langle\psi| + (1-p)|\phi\rangle\langle\phi| \, . \tag{4.9}$$

That is, the density operator ρ allows us to compute any expectation value for the system described above where the system was prepare in the state $|\psi\rangle$ with probability p and state $|\phi\rangle$ with probability $1-p$.

More generally, if a system is prepared in state $|\psi_k\rangle$ with probability p_k it can be described by the density operator

$$\rho = \sum_k p_k |\psi_k\rangle\langle\psi_k| \,.$$

Such states are known as *statistical mixtures* or as *mixed* states. In contrast a state where the exact quantum state is known (i.e. all states studied until now) are known as *pure* quantum states.

How does a generic single qubit mixed state look on the Bloch sphere? To study this we start by recalling Eq. (4.6) and writing

$$\begin{aligned} |\psi\rangle\langle\psi| &= \frac{1}{2}\sigma_0 + \frac{1}{2}\sum_{i=1}^{3} v_i\sigma_i \\ |\phi\rangle\langle\phi| &= \frac{1}{2}\sigma_0 + \frac{1}{2}\sum_{i=1}^{3} u_i\sigma_i \,. \end{aligned}$$

Then we note that the mixed state

$$\begin{aligned} \rho &= p|\psi\rangle\langle\psi| + (1-p)|\phi\rangle\langle\phi| \\ &= \frac{1}{2}\sigma_0 + \frac{1}{2}\sum_{i=1}^{3}(pv_i + (1-p)u_i)\sigma_i \,. \end{aligned}$$

That is, the mixed state has a Bloch vector

$$\mathbf{w} = p\mathbf{v} + (1-p)\mathbf{u} \tag{4.10}$$

composed from the weighted convex combination of the Bloch vectors of the original pure state Bloch vectors. This is when the geometric representation provided by the Bloch sphere really comes into its own. If one already knows the original Bloch vectors, it is basic geometry to sketch the new Bloch vector for the corresponding mixed state (see Fig. 4.1).

While pure states have a Bloch vector of norm 1 and sit on the outside of the Bloch sphere, mixed states fall within the Bloch sphere. This follows immediately from the observation that $\mathbf{w} = p\mathbf{v} + (1-p)\mathbf{u}$. Unless $p = 0$, $p = 1$ or $\mathbf{v} = \mathbf{u}$ (which correspond to pure states), the vector $\mathbf{w}$ will point to some point in the interior of the Bloch sphere with $|\mathbf{w}|^2 = p^2 + (1-p)^2 + 2p(1-p)\mathbf{u}.\mathbf{v} = 1 - 2p(1-p)(1-\mathbf{u}.\mathbf{v}) \leq 1$.

A good physical example of a mixed state is that of a thermal state. A thermal state of a Hamiltonian H at inverse temperature $\beta = 1/k_B T$ can be written as

$$\rho = \frac{e^{-\beta H}}{Z} \tag{4.11}$$

where Z is the partition function of the system $Z = \mathrm{Tr}[e^{-\beta H}]$. To see that this reduces to more familiar notions of the thermal state let us expand it in the eigenbasis of $H = \sum_k E_k |E_k\rangle\langle E_k|$. Using the standard definition of the matrix exponential, in this basis we have

$$\begin{aligned} \rho &= \sum_k e^{-\beta E_k} |E_k\rangle\langle E_k| \\ Z &= \sum_k e^{-\beta E_k} \,. \end{aligned} \tag{4.12}$$

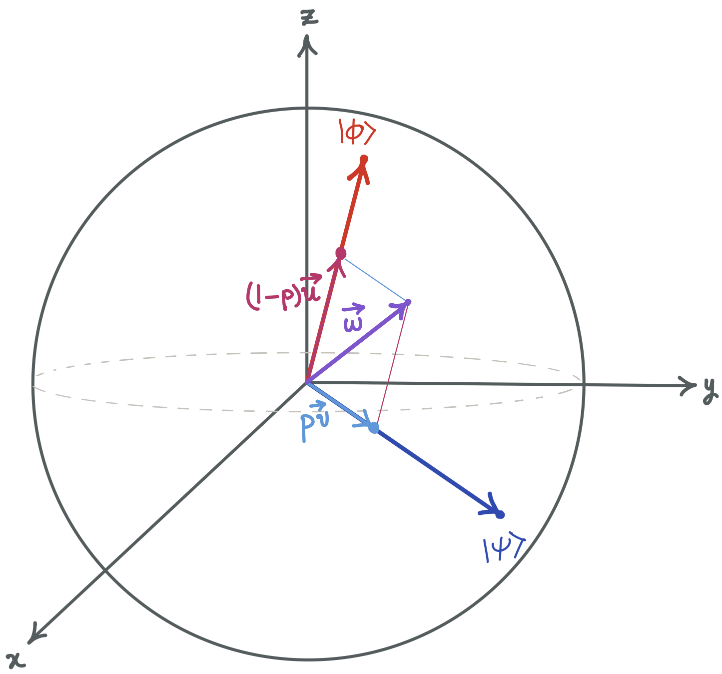


Figure 4.1: **Mixed State.**

That is, ρ corresponds to a mixed state where the energy eigenstate $|E_k\rangle$ is prepared with the probability $p_k = e^{-\beta E_k}/Z$ which should look familiar as the standard Boltzmann distribution from your statistical mechanics courses. The state $\rho = \frac{e^{-\beta H}}{Z}$ can be treated as any quantum state - you can combine it with other quantum states, evolve it unitarily, perform quantum measurements etc etc. Thus we see that the density matrix formalism allows one to combine classical statistical mechanics and quantum mechanics.

4.1.2 Reduced states

In this course so far we have constructed the state of a composite system from the states of the individual systems using the tensor product. But what if one wants to go in the other direction? Say you are given the state $|\Psi\rangle$ of a 4-dimensional system corresponding to two qubits - how could you describe the state of just one of the qubits? If the state of the composite system is a product state, i.e. $|\Psi\rangle = |\psi_A\rangle \otimes |\psi_B\rangle$, this is straightforward, i.e. the state of A is just $|\psi_A\rangle$. But what if $|\Psi\rangle$ is entangled? For example, what if it's the Bell state $|\Psi\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$? Now it's no longer clear how to describe the state of the system A alone. Here we show how this question can be addressed using density operators.

Consider a system composed of two subsystems, A and B, and corresponding Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$. The core idea is to introduce an operator ρ_A (to be defined!) that one can compute from $|\Psi\rangle$ that will allow one to compute all properties of system A alone. That is, given any measurement operator $\hat{O} \otimes \mathbb{1}_B$ that acts non-trivially on A alone, we want to define an operator ρ_A, defined on the Hilbert space of $\mathcal{H}_A$ alone, that will allow one to compute the expectation value of $\hat{O}$.

To identify such an operator let us first write the operator O in its eigenbasis as $O =$

$\sum_{j=1}^{d_A} \lambda_j |\lambda_j\rangle\langle\lambda|_j$. Now we note that the average value of O is given by

$$\langle O\rangle = \sum_{j=1}^{d_A} \lambda_j P_A(\lambda_j) \tag{4.13}$$

where $P_A(\lambda_j)$ is the probability of getting λ_j when measuring system A. Now this probability can be rewritten in terms of

$$P_{AB}(\lambda_j, k) = \langle\lambda_j k|\rho_{AB}|\lambda_j k\rangle\,, \tag{4.14}$$

the joint probability of finding A to be in $|\lambda_j\rangle$ and system B to be in the state computational basis state[1] $|k\rangle$. Concretely, we have

$$P_A(\lambda_j) = \sum_{k=1}^{d_B} P_{AB}(\lambda_j, k) = \sum_{k=1}^{d_B}\langle\lambda_j k|\rho_{AB}|\lambda_j k\rangle\,. \tag{4.15}$$

Thus we have

$$\begin{aligned}\langle O\rangle &= \sum_{j=1}^{d_A} \lambda_j \sum_{k=1}^{d_B}\langle\lambda_j k|\rho_{AB}|\lambda_j k\rangle \\ &= \sum_{j=1}^{d_A} \lambda_j\langle\lambda_j|\left(\sum_{k=1}^{d_B}(\mathbb{I}_A\otimes\langle k|)\rho_{AB}(\mathbb{I}_A\otimes|k\rangle)\right)|\lambda_j\rangle \\ &= \sum_{j=1}^{d_A} \lambda_j\langle\lambda_j|\rho_A|\lambda_j\rangle \\ &= \mathrm{Tr}[\rho_A O]\end{aligned} \tag{4.16}$$

where we have defined

$$\rho_A := \sum_{k=1}^{d_B}(\mathbb{I}_A\otimes\langle k|)\rho_{AB}(\mathbb{I}_A\otimes|k\rangle) \equiv \mathrm{Tr}_B[\rho_{AB}] \tag{4.17}$$

This operator is known as a *reduced state* and is another type of density operator. Note that since the trace of an operator is invariant under a change of basis, the use of a density operator to calculate the average value of $\hat{O}$ does not depend on the choice of the basis used to define this operator.

It is worthwhile becoming fluent at taking the partial trace of a quantum state. This is usually easiest to do using braket notation rather than working with the explicit matrix forms. To do so, it's helpful to note (prove this to yourself!) that:

$$\mathrm{Tr}_B[|ij\rangle\langle kl|] = |i\rangle\langle k|\,\mathrm{Tr}[|j\rangle\langle l|] \tag{4.18}$$

from which point you can make use of the standard properties of the trace (e.g. cyclicity).

Example 4.1.2. The reduced state of $|\psi_A\psi_B\rangle$ is given by the density operator $\rho_A = |\psi_A\rangle\langle\psi_A|$ as one would expect from our arguments at the start:

$$\begin{aligned}\rho_A &= \mathrm{Tr}_B[|\psi_A\psi_B\rangle\langle\psi_A\psi_B|] \\ &= |\psi_A\rangle\langle\psi_A|\mathrm{Tr}_B[|\psi_B\rangle\langle\psi_B|] \\ &= |\psi_A\rangle\langle\psi_A|\langle\psi_B|\psi_B\rangle \\ &= |\psi_A\rangle\langle\psi_A|\,.\end{aligned} \tag{4.19}$$

[1] This choice in basis is arbitrary. Any orthogonal basis will do.

Example 4.1.3. Consider the Bell state $|\Phi_+\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle$. The reduced state on qubit A is given by

$$\begin{aligned}\rho_A &= \mathrm{Tr}_B[|\Phi^+\rangle\langle\Phi^+|] \\ &= \frac{1}{2}\mathrm{Tr}_B[|00\rangle\langle 00| + |00\rangle\langle 11| + |11\rangle\langle 00| + |11\rangle\langle 11|] \\ &= \frac{1}{2}(|0\rangle\langle 0|\mathrm{Tr}[|0\rangle\langle 0|] + |0\rangle\langle 1|\mathrm{Tr}[|0\rangle\langle 1|] + |1\rangle\langle 0|\mathrm{Tr}[|1\rangle\langle 0|] + |1\rangle\langle 1|\mathrm{Tr}[|1\rangle\langle 1|]) \\ &= \frac{1}{2}(|0\rangle\langle 0|\langle 0|0\rangle + |0\rangle\langle 1|\langle 0|1\rangle + |1\rangle\langle 0|\langle 0|1\rangle + |1\rangle\langle 1|\langle 1|1\rangle) \\ &= \frac{1}{2}(|0\rangle\langle 0| + |1\rangle\langle 1|) \\ &= \frac{1}{2}\mathbb{1}\end{aligned} \tag{4.20}$$

That is, the reduced state on qubit A is the *maximally mixed* state where with equal probability the qubit is in state 0 or state 1. Similarly, $\rho_B = \frac{1}{2}\mathbb{1}$. Crucially we note that

$$\begin{aligned}\rho_A \otimes \rho_B &= \frac{1}{2}\left(|00\rangle\langle 00| + |01\rangle\langle 01| + |10\rangle\langle 10| + |11\rangle\langle 11|\right) \\ &\neq |\Phi^+\rangle\langle\Phi^+|\,.\end{aligned} \tag{4.21}$$

Thus we see that if you look at only one half of a Bell state the statistical outcomes are no different to tossing a fair coin. But the state of two fair coins is not the same as a Bell state. The interesting behaviour of a Bell state can only be captured by studying the correlations between both systems and captured by the pure state $|\Phi^+\rangle$.

Exercise: Use the notion of a reduced state to argue that entanglement cannot be used for faster than light signalling.

4.1.3 General properties of density operators

Above we have presented two different ways of obtaining mixed state density operators: by direct construction or as the reduced state of a larger system. More generally, density operators can be introduced more abstractly as any operator with the following properties.

Property 4.1.4. *1. The density operator is self-adjoint, that is to say,* $\rho_A^\dagger = \rho_A$*,*

2. $\mathrm{Tr}(\rho_A) = \sum_i \rho_{ii} = \sum_{i,\mu} |\alpha_{i,\mu}|^2 = \|\psi\|^2 = 1$*,*

3. The density operator is positive semidefinite, i.e. $\langle\phi|\rho_A|\phi\rangle \geq 0$ *for all* $|\phi\rangle \in A$*.*

It is straightforward to show that the reduced states introduced above satisfy these properties.

Demo. 1. We have:

$$\begin{aligned}\rho_{ij} &= \sum_\mu \alpha^*_{i,\mu}\alpha_{j,\mu} \\ \rho_{ji} &= \sum_\mu \alpha^*_{j,\mu}\alpha_{i,\mu}\end{aligned}$$

One should see that

$$\rho_{ij} = \overline{\rho_{ji}}$$

2. We compute:

$$\sum_i \rho_{ii} = \sum_i \sum_\mu \alpha^*_{i,\mu}\alpha_{i,\mu} = \sum_i \sum_\mu \langle i\mu|\psi\rangle\langle\psi|i\mu\rangle$$
$$= \sum_{i,\mu} |\langle i\mu|\psi\rangle|^2$$

The $|i\rangle$ and $|\mu\rangle$ form a basis of A and B, respectively. Thus, the sum over i and μ give the norm of $|\psi\rangle$, which is by definition normalized to 1.

3. We compute :

$$\begin{aligned}\langle\phi|\rho_A|\phi\rangle &= \sum_{i,j}\sum_\mu \langle\phi|i\rangle\langle j|\phi\rangle\langle i\mu|\psi\rangle\langle\psi|j\mu\rangle \\ &= \sum_\mu \beta_\mu\beta^*_\mu \\ &= \|\beta\|^2 \geq 0,\end{aligned}$$

where $\beta_\mu = \langle\phi|i\rangle\langle i\mu|\psi\rangle$

□

Notice that these properties imply, in particular:

- There exists a basis in which ρ_A is diagonal (from point 1),
- Furthermore, points 2 and 3 impose a particular form on the diagonal representation of the operator ρ_A:

$$\rho_A = \sum_j p_j |j\rangle\langle j|,$$

where $p_j \geq 0$ and $\sum p_j = 1$. Thus,

$$\langle\hat{O}\rangle = \mathrm{Tr}(\rho_A\hat{O}) = \sum_j p_j \langle j|\hat{O}|j\rangle = \sum_j p_j \langle\hat{O}\rangle_{|j\rangle},$$

where $\langle\hat{O}\rangle_{|j\rangle}$ denotes the average value of $\hat{O}$ for the subsystem consisting of state $|j\rangle$.

We note that if a density operator describes a pure state, then it is a projector, i.e., $\rho^2 = \rho$. In fact, the two properties are equivalent: if $\rho^2 = \rho$, the eigenvalues of the density operator must necessarily be 0 or 1. But since the sum of the eigenvalues of a density operator must be equal to 1, there must be a single eigenvalue of the density operator that equals 1, and it is unique.

On the other hand, if ρ is not pure then we have $\rho^2 \neq \rho$ and $\mathrm{Tr}[\rho^2] \leq 1$. To see this we consider writing in its eigenbasis as $\rho = \sum_k \lambda_k|\psi_k\rangle\langle\psi_k|$. It follows that $\rho^2 = \sum_k \lambda_k^2|\psi_k\rangle\langle\psi_k| \neq \rho$ and $\mathrm{Tr}[\rho^2] = \sum_k \lambda_k^2$ and this is less than 1 unless $\{\lambda_k\} = \{1, 0\}$ which again reduces to the case where $\rho = |\psi_0\rangle\langle\psi_0|$ is a pure state. The quantity $\mathrm{Tr}[\rho^2]$ is known as the *purity* of a state - it takes its maximal value of 1 for a pure state and is less than 1 otherwise. An alternative way of showing that mixed states live within the interior of the Bloch sphere is to establish that the condition that $\mathrm{Tr}[\rho^2] \leq 1$ implies that the norm of the Bloch vector is less that 1, i.e. $|\mathbf{w}| \leq 1$. We leave this as an exercise for the reader.

4.1.4 Evolution of density operators

Let's consider a density operator in diagonal form at $t = 0$:

$$\rho(t = 0) = \sum_j \alpha_j \left|\psi_j(0)\right\rangle \left\langle\psi_j(0)\right|$$

We are interested in determining the laws governing its time evolution. We assume that the statistical mixture does not change over time. In other words, α_i does not depend on t, and

$$\rho(t) = \sum_j \alpha_j \left|\psi_j(t)\right\rangle \left\langle\psi_j(t)\right|.$$

The time evolution of a state has already been characterized as:

$$\left|\psi_j(t)\right\rangle = e^{-iHt} \left|\psi_j(0)\right\rangle$$

Using these two equations, we obtain:

$$\rho(t) = \sum_j \alpha_j e^{-iHt} \left|\psi_j(0)\right\rangle \left\langle\psi_j(0)\right| e^{iHt}$$

We differentiate:

$$\begin{aligned}\frac{\partial\rho}{\partial t} &= \sum_j \alpha_j \left(-iH\right) e^{-iHt} \left|\psi_j(0)\right\rangle \left\langle\psi_j(0)\right| e^{-iHt} \\ &+ \sum_j \alpha_j e^{-iHt} \left|\psi_j(0)\right\rangle \left\langle\psi_j(0)\right| \left(iH\right) e^{-iHt} \\ &= \left(-iH\right)\rho + \rho\left(iH\right)\end{aligned}$$

which leads to the equation:

$$i\frac{\partial\rho}{\partial t} = -[\hat{H}, \rho], \tag{4.22}$$

describing the time evolution of the density operator. Note that while this may look like the Heisenberg equation, ρ does not define an observable physical quantity!

Chapter 5

Measurement and decoherence

5.1 The measurement problem

Here we will discuss a topic at the very core of quantum mechanics that is fundamental to our understanding (/lack of understanding) of the field known as the measurement problem.

The measurement problem can be set up from the following basic assumptions about the theory of quantum mechanics.

1. Basic Conception of a measuring device: a good measuring device is accurate.
2. Quantum Mechanics is a universal and fundamental theory
3. Weak Physicalist Postulate: The description of the behaviour of large objects must be consistent with the laws governing the behaviour of the smaller objects of which they consist.

A quantum measuring device is a device which can extract information from a quantum system. A basic measuring device, e.g. for measuring the spin state of an electron, can be envisioned as follows. The device has a pointer and three possible positions labelled "ready", "up" and "down". The pointer is at "ready" initially. In order for the measuring device to be accurate we simply require that the device can correctly inform us of the state of the electron. As such, we require that when an "up electron" is fed in the pointer moves from the "ready" label to the "up" label. When a "down electron" is fed in, the pointer moves from the "ready" label to the "down" label. That is, we have

$$\begin{aligned} &|\text{'ready'}\rangle_M |\uparrow\rangle_S \rightarrow |\text{'up'}\rangle_M |\uparrow\rangle_S \\ &|\text{'ready'}\rangle_M |\downarrow\rangle_S \rightarrow |\text{'down'}\rangle_M |\downarrow\rangle_S \end{aligned} \tag{5.1}$$

Then from assumptions 2. and 3. we get that we should be able to describe our measuring device quantum mechanically. Thus, we should ascribe quantum mechanical states to the measurement system's pointer states.

Based on these assumptions the following is a simple way of setting up the measurement problem. We start with the following postulates of quantum mechanics.

(A) **Formalism:** Every physical quantity is represented by an operator Q and every state of a physical system by a state vector $|\psi\rangle$

(B) **Measurement Kinematic Postulate:** If a quantity Q is measured, the post measurement state of the system will be the eigenstate corresponding to the eigenvalue measured.

(C) **Dynamical Postulate:** Time evolution is a linear map from state to state.

Consider measuring the spin of an electron using the accurate measurement device outlined above. A contradiction is generated when we consider what happens when you feed a superposition into the measuring device. That is, suppose we feed in

$$|\text{'ready'}\rangle_M \frac{1}{\sqrt{2}}(|\uparrow\rangle_S + |\downarrow\rangle_S) \tag{5.2}$$

Given our conception of a good measuring device (Eq. (5.5)) and that, from the Dynamical Postulate, quantum systems evolve linearly, the resulting state is

$$|\text{'ready'}\rangle_M \frac{1}{\sqrt{2}}(|\uparrow\rangle_S + |\downarrow\rangle_S) \to \frac{1}{\sqrt{2}}(|\text{`up'}\rangle_M|\uparrow\rangle_S + |\text{`down'}\rangle_M|\downarrow\rangle_S) \tag{5.3}$$

We are left with a superposition of the measurement device being in the 'up' state and the 'down' state.

In this way the linearity of quantum mechanics dynamics combined with quantum mechanical treatment of a basic conception of a measuring device leads to the conclusion that a system in a superposition remains in a superposition. According to dynamical postulate there is no way to get the system into an eigenstate of an observable if it is not already in one. However, this contradicts A! The Measurement Kinematic Postulate states that post measurement of the system will be in an eigenstate of the observable being measured.

So, can we just get rid of the Measurement Kinematic Postulate to solve the measurement problem? Not quite. There are still many conceptual problems with how to understand Eq. (5.3).

(i) It seems to **contradict with the world around us** - we don't seem to see these weird macroscopic superpositions between measurement devices.

(ii) It seems to **contradict quantum formalism**, in particular, the Born rule.

5.2 Easy resolutions and why they do not solve the problem

5.2.1 The collapse postulate

Doesn't the collapse postulate resolve the measurement problem? Von Neumann claimed that there must be two fundamental laws about how the states of Quantum Mechanics evolve.

(I) When no measurements are going on, the states of all physical systems evolve linearly (via the Schrodinger equation) in accordance with the dynamical postulate.

(II) When there are measurements, the systems do not evolve in accordance with the dynamical equations of motion. Instead, they evolve in accordance with the postulate of collapse.

Criticism: The problem with this approach is that the word measurement does not have a precise enough meaning to play such a fundamental role in the laws of physics. As such, these rules do not determine exactly how the world behaves and so do not amount to fundamental laws. (This contradicts premise 2 in the first part of this note).

Figure 5.1: Credit: L'heure est grave

In particular, there are two key ambiguities with the term measurement.

Firstly, *what processes count as measurements?* A measurement is something which extracts information from a system. However, many actions not conventionally associated with measurement extract information from a system. If observing a dead cat tells you that an electron must have "spin up" or else it would not have been able to set off the killing device, then observing the dead cat is a measurement. Seen in this way measurement are made continually and so we are lead to the conclusion that all most all evolution takes place via the collapse postulate rather than quantum mechanics. However, Quantum Mechanics cannot be driven just by rule II because that tells us nothing about how systems evolve with time and states clearly do evolve.

Secondly, *measurement requires a divide between the system being measured and the part doing the measuring and there is no definite prescription for how this division is to be made.* John Bell in his essay *"Against Measurement"* uses the example of an alpha particle travelling along a photographic plate. We can either consider the alpha particle as the system and the photographic plate as the external measuring device or we can consider the photographic plates as also part of the quantum mechanical system. The two records are mutually consistent and though the second is more detailed than the first it is clearly not the final description. Given these considerations how can we apply Von Neumann's two rules? Does rule I cease to apply as soon as the alpha particle reaches the photographic plate, when the temperature of the cloud chamber rises, when I take a photo or when this photo is observed? Bell advocates the guiding rule: "put the split sufficiently much into the quantum system that the inclusion of more would not significantly alter practical purposes". This rule is sufficiently unambiguous for practical purposes though it is still fundamentally ambiguous.

5.2.2 Decoherence

A more modern way of at least in part resolving the measurement problem is via the concept of decoherence. Note that decoherence is a fundamental physical phenomenon that is important to understand independently of the measurement problem.

Core to understanding decoherence is the observation that the environment acts a good measurement device. This means that corresponding to different positions of the electron are environmental 'pointer' states such as "the total environment as if the electron is at x". (Even in the absence of matter, radiation reflecting from an electron records its location and this radiation will in turn causally interact with its surroundings.) Thus, treating the environment as a measurement device, we can generalize Eq. (5.5) and write

$$\begin{aligned}
&|\text{`Initial Environment'}\rangle_E|\text{'ready'}\rangle_M|\uparrow\rangle_S \to |\text{`Total environment given}\uparrow'\rangle_E|\text{`up'}\rangle_M|\uparrow\rangle_S \\
&|\text{`Initial Environment'}\rangle_E|\text{'ready'}\rangle_M|\downarrow\rangle_S \to |\text{`Total environment given}\downarrow'\rangle_E|\text{`down'}\rangle_M|\downarrow\rangle_S
\end{aligned} \tag{5.4}$$

And so the output state after the measurement and interaction with the environment will be

$$|\psi^{\text{out}}\rangle_{EMS} \propto |\text{`Total environment given}\uparrow'\rangle_E|\text{`up'}\rangle_M|\uparrow\rangle_S + |\text{`Total environment given}\downarrow'\rangle_E|\text{`down'}\rangle_M|\downarrow\rangle_S \tag{5.5}$$

Now if we look at the reduced state on the system and measurement device will be

$$\begin{aligned}
\rho_{MS}^{\text{decoh}} &= \text{Tr}_E[|\psi^{\text{out}}\rangle\langle\psi^{\text{out}}\rangle_{EMS}|] \\
&= \frac{1}{2}\left(|\text{`up'}\rangle\langle\text{`up'}|_M + |\text{`down'}\rangle\langle\text{`down'}|_M + r|\text{`up'}\rangle\langle\text{`down'}|_M + r^*|\text{`down'}\rangle\langle\text{`up'}|_M\right) .
\end{aligned} \tag{5.6}$$

where $r = \langle\text{`Total environment given}\uparrow'|\text{`Total environment given}\downarrow'\rangle$.

In the realistic limit where $r \to 0$ we then have:

$$\rho_{MS}^{\text{decoh}} \to \rho_{MS}^{\text{Born}} := \frac{1}{2}\left(|\text{`up'}\rangle\langle\text{`up'}|_M + |\text{`down'}\rangle\langle\text{`down'}|_M\right) \tag{5.7}$$

where ρ_{MS}^{Born} is the state you would expect to get out from measurement corresponding to the case where you find the spin either in the up or down state with equal probabilities.

What does this tell us? Well this largely deals with the worry that states like Eq. (5.3) contradict with the world around us. It explains why we do not observe interference between macroscopic objects like measurement devices.

Does it also solve the contradiction with the Born rule? Not really. And that's because even those we find that $\rho_{MS}^{\text{decoh}} = \rho_{MS}^{\text{Born}}$ mathematically there is an important difference between what the states on the left and right sides of this equality represent conceptually physically. This is the distinction between proper and improper mixtures.

Proper mixtures: Mixed states that can be interpreted as arising from ignorance of the underlying pure state.

Improper mixtures: Mixtures that arise when you examine a subsystem of a larger pure state.

The state resulting from decoherence ρ_{MS}^{decoh} is an improper mixture (i.e. that formed from a reduced state), where as the state captured by the Born rule ρ_{MS}^{Born} is a proper mixture. Therefore they do not represent the same physical scenario despite being represented by the same mathematical entity. (Note, this mathematical equivalence/ambiguity is why we can forget about the measurement problem when getting on with life/research most of the time).

Sometimes the measurement problem is stated directly in terms of proper and improper mixtures as the contradiction that the Born rule says the outcome of a measurement is a proper mixture but the output of a measurement according to the dynamical laws of quantum mechanics is an improper mixture.

5.2.3 Instrumentalism

It is sometimes suggested that the measurement problem can be avoided by taking an instrumentalist approach to quantum mechanics.

The proposed solution is typically to deny assumption 2 right at the start, namely that quantum mechanics is a 'universal and fundamental theory'. Instead it is claimed that the wavefunction depends on the knowledge of the person doing the calculation. Individuals with different amounts of knowledge concerning the system will come up with different wavefunctions. This is why the wavefunction appears to "collapse" when the measurement device is read. If we have an accurate measuring device and the device reads "up" we can infer that the pointer state of the device is "up" and the electron is spin up. The change is non linear because our knowledge changes but this is unproblematic we are treating our knowledge as external to rather than part of the dynamic process.

Criticism: To start, it is worth asking whether the approach advocated here is one of limited or universal instrumentalism. Either answer is problematic. If the instrumentalism is limited just to the wavefunction - then it needs to be asked whether this limitation is coherent and warranted. That is, why are we treating the wavefunction differently to other concepts in physics. If the instrumentalism is universal then all the usual reasons for thinking instrumentalism is an untenable philosophical position apply (see https://plato.stanford.edu/entries/scientific-realism/ for a long discussion).

The measurement problem is a fundamental problem in quantum mechanics that really gets at the essence of what the theory tells us about the nature of the world. Nonetheless, it is one that we can largely ignore while getting on with most research (and passing most exams).

However, if I have sparked your attention and you are interested in reading more about the measurement problem I would first recommend reading *"Against Measurement"* by John Bell. There he argues that quantum mechanics is a theory of observables rather than beables. Quantum mechanics is entirely concerned with "the results of measurements"; however, the concept of measurement becomes so vague on reflection that it is unsatisfying to have it at the centre of a fundamental theory. Quantum mechanics divides the world into two parts; that which is observed and that which is observing. The results depend on how this division is made but only a practical guide can be given on where to draw the line. His proposed solution: such a theory cannot be complete.

If you would then like to read about some more modern potential resolutions of the measurement problem I would recommend reading David Wallace on the Many Worlds interpretation and Carlo Rovelli on quantum relationalism.

5.3 Decoherence as a dynamical process

This section is a lightly modified version of Jim Al-Khalili's notes on decoherence which are available at https://www.surrey.ac.uk/sites/default/files/2023-01/introduction-to-decoherence-theory-lectures-one-to-five.pdf and I copy here for convenience.

Two limits of quantum measurement

The total Hamiltonian of a system and environment can be written as

$$H_{SE} = H_S \otimes \mathbb{I} + \mathbb{I} \otimes H_E + \lambda H_I \,. \tag{5.8}$$

In the limit in which the interaction energy is small (i.e. broadly when λ is small compared to the eigenenergies of H_S and H_E) we can ignore the interaction term and we have that the system and environment evolve under H_S and H_E independently:

$$\begin{aligned} e^{-itH_{SE}}|\psi_S\phi_E\rangle &\approx e^{-itH_S\otimes\mathbb{I}+\mathbb{I}\otimes H_E}|\psi_S\phi_E\rangle \\ &= e^{-itH_S\otimes\mathbb{I}}e^{-it\mathbb{I}\otimes H_E}|\psi_S\phi_E\rangle \\ &= e^{-itH_S}\otimes e^{-itH_E}|\psi_S\phi_E\rangle \\ &= e^{-itH_S}|\psi_S\rangle \otimes e^{-itH_E}|\phi_E\rangle \,. \end{aligned} \tag{5.9}$$

This is implicitly what has been assumed in most (all?) calculations you have performed previously. For example, when we studied the two slit experiment we did not model the interaction between the system and the environment.

What happens if we instead consider the limit in which the interaction term dominates?

We often write the interaction Hamiltonian as $H_I = S \otimes E$, where S and E are operators acting in the Hilbert spaces of the system and environment. We really only need to worry about S which will correspond to some system observable like its position that is superselected by the environment (i.e., constantly being monitored by the environment).

Let's suppose, as is the case very often in practise, that the system and environment interact in the position basis. That is, let

$$H_I = \hat{x} \otimes \hat{E} \tag{5.10}$$

where

$$\hat{x} = \sum_i x_i |X_i\rangle\langle X_i|, \tag{5.11}$$

and x_i are position eigenvalues and $|X_i\rangle$ are position eigenstates. (Note the above equation defining the operator is just the equivalent of the eigenvalue equation $\hat{x}|X_i\rangle = x_i|X_i\rangle$). It then follows that since system and environment operators act in different Hilbert spaces we have that

$$[H_I, \hat{x}] = (\hat{x} \otimes \hat{E})\hat{x} - \hat{x}(\hat{x} \otimes \hat{E}) = \hat{x}\hat{x} \otimes \hat{E} - \hat{x}\hat{x} \otimes \hat{E} = 0 \tag{5.12}$$

This commutation relation is known as Zurek's commutativity criterion. Therefore, while in general the position operator does not commute with the total Hamiltonian (i.e. we cannot measure the position and energy of a quantum system simultaneously) it holds in this particular limit (the quantum measurement limit) of $\hat{H} = \hat{H}_I = \hat{x} \otimes \hat{E}$. So, $\hat{H}_I$ and $\hat{x}$ have common eigenstates, $|X_i\rangle$.

If we start the system in some position eigenstate, $|X_i\rangle$, and the environment in initial state, $|E_0\rangle$, then at $t = 0$ the combined state is $|X_i\rangle|E_0\rangle$. An evolution operator, $\hat{U}$, will take this forward to time t:

$$\hat{U}|X_i\rangle|E_0\rangle = e^{-i\hat{H}_I t}|X_i\rangle|E_0\rangle = |X_i\rangle e^{-ix_i\hat{E}t}|E_0\rangle = |X_i\rangle|E_{x_i}\rangle, \quad (4.17) \tag{5.13}$$

where $|E_{x_i}\rangle$ is the state of the environment now containing information about the position of the quantum system (particle).

What we see in this last equation is that the system and environment are still not entangled. So $|X_i\rangle$ represents an *environmentally superselected preferred state.* Let our system be in a superposition of pointer states:

$$|\psi\rangle = \sum_i c_i|X_i\rangle. \quad (4.18) \tag{5.14}$$

Now

$$e^{-i\hat{H}_I t}|\psi\rangle|E_0\rangle = e^{-i\hat{x}\otimes\hat{E}}\left(\sum_i c_i|X_i\rangle\right)|E_0\rangle$$

$$= \left(c_1|X_1\rangle e^{-ix_1\hat{E}t} + c_2|X_2\rangle e^{-ix_2\hat{E}t} + \cdots\right)|E_0\rangle$$

$$\to c_1|X_1\rangle|E_1(t)\rangle + c_2|X_2\rangle|E_2(t)\rangle + \cdots,$$

where we now have an entangled state of system and environment and $|E_1\rangle$ etc is the state of the environment that contains information about the system being in position x_1. If these states are close to orthogonal, i.e. $\langle E_i(t)|E_j(t)\rangle \to 0$ then the reduced state of the system will be completely decohered in the position basis.

Note there was nothing special persay about the position basis, we could have run this argument in any basis and that would lead to decoherence in *that* basis. However, the basis of decoherence it determined by the form of the interaction Hamiltonian. And that will typically, but not always, be the position basis.

5.3.1 A simple model for decoherence

Physical systems exhibiting decoherence are varied. Luckily – and perhaps surprisingly – a small set of simple canonical models can describe a wide range of phenomena and physical systems. Thus the system of interest can be modelled as either a spin-$\frac{1}{2}$ particle (qubit) or as having continuous phase space variables and moving in some potential (H-O or double well are popular examples). The environment likewise can be modelled either as a collection of qubits or as a heat bath of harmonic oscillators.

Consider a quantum system S to be a qubit with basis states $|0\rangle$ and $|1\rangle$ denoting spin up and down with respect to the z-axis. The total system plus environment is described by a tensor product Hilbert space

$$H = H_S \otimes H_{e_1} \otimes H_{e_2} \otimes \cdots \otimes H_{e_N}, \tag{5.15}$$

where H_S denotes the Hilbert space of the system and H_{e_i} denotes the Hilbert space of the i-th environmental qubit.

The total Hamiltonian is chosen to be of the form

$$H = H_I = \frac{1}{2}\hat{\sigma}_z \otimes \left(\sum_{i=1}^{N} g_i^{(i)}\hat{\sigma}_z^{(i)}\right) = \frac{1}{2}\hat{\sigma}_z \otimes \hat{E}. \tag{5.16}$$

where g_i are coupling strengths and $\hat{\sigma}_z^{(i)}$ is a Pauli Z on the $i_{\rm th}$ environment qubit (for compactness of notation I am suppressing a bunch of identity operators on the other environment qubits but technically they should be there).

Now, when we act with the evolution operator involving the above Hamiltonian on an initial unentangled state of system and environment we see

$$e^{-i\hat{H}_I t}|0\rangle|E_0\rangle = e^{-\frac{i}{2}\hat{\sigma}_z\otimes\hat{E}t}|0\rangle|E_{\rm initial}\rangle = |0\rangle e^{-\frac{i}{2}\sum_i g_i\hat{\sigma}_z^{(i)}t}|E_{\rm initial}\rangle = |0\rangle|E_0(t)\rangle, \tag{5.17}$$

where the state of the environment can start off as complicated as we wish, with each qubit in a superposition:

$$|E_{\rm initial}\rangle = (\alpha_1|0\rangle + \beta_1|1\rangle)\otimes\ldots\otimes(\alpha_N|0\rangle + \beta_N|1\rangle)\,. \tag{5.18}$$

Thus we see that in this case the state remains a product state.

If instead the system starts off in a superposition then

$$e^{-iH_{\rm int}t}(\alpha|0\rangle + \beta|1\rangle)|{\rm E}_{\rm initial}\rangle \to \alpha|0\rangle|{\rm E}_0(t)\rangle + \beta|1\rangle|{\rm E}_1(t)\rangle \tag{5.19}$$

where $|{\rm E}_0(t)\rangle := e^{-\frac{i}{2}\sum_i g_i\hat{\sigma}_z^{(i)}t}|E_{\rm initial}\rangle$ and $|{\rm E}_1(t)\rangle := e^{\frac{i}{2}\sum_i g_i\hat{\sigma}_z^{(i)}t}|E_{\rm initial}\rangle$.

We have seen already that the rate of decoherence depends on the overlap of the environment states that are entangled with each of the system states and the degree to which they are orthogonal (distinguishable)

$$r(t) = \langle{\rm E}_1(t)|{\rm E}_0(t)\rangle. \tag{5.20}$$

To get a handle on this let us first note that we can write the environment states more compactly as

$$|{\rm E}_0(t)\rangle = \sum_{j=1}^{2^N} e^{-ie_jt/2}c_j|n_j\rangle. \tag{5.21}$$

where we switch to binary notation, i.e. $|n_0\rangle = |00...0\rangle$, $|n_1\rangle = |00...1\rangle$ etc. The c_j coefficients are each a product of N α's and β's (for example, $c_1 = \alpha_1\alpha_2\cdots\alpha_N$); and finally, the energy e_j is

$$e_j = \sum_{k=1}^{N}(-1)^{n_j}g_k, \quad n_j = \begin{cases} 0 & \text{for an even number of } |1\rangle \text{ states in the product } |n_j\rangle \\ 1 & \text{for an odd number of } |1\rangle \text{ states in the product } |n_j\rangle \end{cases} \tag{5.22}$$

Now we can look at the overlap of two environment states to see the structure of the decoherence rate r. The two environment states only differ by a sign in the exponent and therefore, taking the overlap means we have two minus signs

$$r(t) = \langle{\rm E}_1(t)|{\rm E}_0(t)\rangle = \sum_{i,j}^{2^N} e^{-ie_jt/2}e^{-ie_it/2}c_i^*c_j\langle n_i|n_j\rangle = \sum_{i=1}^{2^N} e^{-ie_it}|c_i|^2. \tag{5.23}$$

It was shown by Zurek in his classic paper (Phys. Rev. D 26, 1862 (1982)) that evolution of $r(t)$ reduces to a random walk problem in the 2-D complex plane and that the time averaged modulus square of the complex vector $r(t)$ scales as

$$\langle|r(t)|^2\rangle \propto 2^{-N} \quad \text{as} \quad t\to\infty \tag{5.24}$$

That is, the rate of decoherence scales exponentially with the size of the environment. We will not prove this here but you can clearly see how the size of the environment affects the decoherence rate since recall that the c_i coefficients in Eq.(5.15) are each a product of N amplitudes, α and β. That is $|c_i|^2$ is a product of N probabilities, each < 1. So the larger the environment (size of N), the smaller the value of $|c_i|^2$ in (5.14).

For very large N, the decoherence rate is roughly a Gaussian decay:

$$r(t) \approx e^{-\Gamma^2 t^2}. \tag{5.25}$$

The decay constant, Γ^2, depends on the distribution of the coupling strengths, g_i, between the system and each of the qubits in the environment. You see, for our model, each of the 2^N terms in the sum in (5.15) a different phase since e_j is a sum (Eq.(5.12)) of coupling strengths whose sign depends on whether the qubit in the environment is spinning up or down.

Decoherence versus dissipation The relaxation time t_r is defined as the time taken for a system to dissipate thermal energy into its environment until they reach thermal equilibrium. However, decoherence can occur even without energy dissipation, meaning the environment can gain information about the system without energy exchange. Decoherence typically takes place on a faster time scale than dissipation/thermalization; however this is problem dependent.

Decoherence versus classical noise Classical noise and decoherence represent different physical processes. Classical noise can in principle be undone by local operations and is very slow. In contrast, decoherence is a process where the system perturbs the environment, leading to a fast, effectively irreversible process.

Chapter 6

Quantum Computing

Computers are fundamentally machines based on physical processes. The physics of these systems is governed by the laws of quantum mechanics. One can thus consider every computer as being "quantum." In reality, this is not the case: their operations can be ideally described by elements of classical physics. For example, Alan Turing constructed a basic computer, the Turing machine, using mechanical components (and following purely classical considerations). A genuinely quantum computer fully utilizes specifically quantum phenomena (such as entanglement) that have no classical equivalent [1].

We are in the middle of a world wide race to build such devices with start ups, tech giants (Google, IBM, Microsoft) all pouring millions into developing such devices. Currently the available devices are analogous to vacuum tube classical computers built in the 1950s and no one has yet to build a device that can implement a genuinely useful algorithm (i.e something that cannot be done better classically). But we're getting to the point where someone might. In fact, people keep on claiming to and then someone else finds a way of doing what they have done classically [2]. So it is realistic that I might need to update these notes before not so long.

In parallel to the hardware efforts, a large community has been working on quantum algorithms to implement on quantum hardware. Here we will give a very brief introduction to this framework. However, to learn more I would recommend Vincenzo Savona's Introduction to Quantum Computing course.

6.1 Quantum Circuits

In contrast to last week where we discussed how realistically all systems interact with their environment, the field of quantum computing relies on the ability to well isolate a system from its environment (this is what makes developing large devices that can do anything useful so hard!). Assuming this isolation is successful, the only evolution is unitary evolution governed by the Hamiltonian

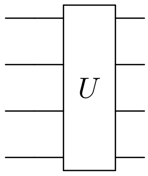
$$|\Psi(t)\rangle = \hat{U}(t,t')\,|\Psi(t')\rangle$$

$$\hat{U}(t,t') = e^{-i\frac{\hat{H}(t-t')}{\hbar}}$$

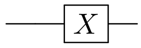
[1] This definition will do for now but a precise definition of a quantum computer is surprisingly hard to pin down. If you're looking to procrastinate check out this twitter thread which (like many a good internet argument) rapidly derails.

[2] Again twitter is great to follow this back and forth.

For a system of N qubits, a quantum operation can be illustrated by a quantum circuit:



Each line represents the state of a qubit. This representation is due to the fact that a unitary operation U is completely defined (by linearity) by its action on the elements of the basis of $\mathcal{H}_N$. Knowing how U acts on $|\alpha_1, \cdots, \alpha_N\rangle$, where $\alpha_i = 0, 1$, is enough to define U completely. For example, consider the NOT gate:

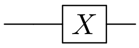
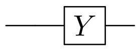
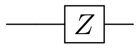
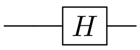
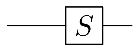
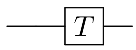


which can be rewritten in vector form with $|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $|1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$:

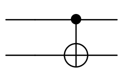
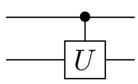
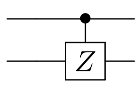
$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

(which is also the Pauli matrix σ_x). This gate maps $|0\rangle$ ($|1\rangle$) to $|1\rangle$ ($|0\rangle$). Its action on an arbitrary state $|\Psi\rangle$ follows from linearity.

Let's list some useful **single qubit** quantum gates [3]:

X		$X = \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$
Y		$Y = \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$
Z		$Z = \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$
Hadamard		$H = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$
Phase		$S = \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix}$
$\frac{\pi}{8}$		$T = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{pmatrix} = e^{i\pi/8} \begin{pmatrix} e^{-i\pi/8} & 0 \\ 0 & e^{i\pi/8} \end{pmatrix}$

And here are some useful **two qubit** quantum gates:

$CNOT$		$C_{NOT} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$
$C - U$ general controled gate		$\|c\rangle \otimes \|x\rangle \to \|c\rangle \otimes U^c \|x\rangle$
$C - Z$ example of controled gate		$C - Z = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$

[3] Continuing the theme of quantum information theorists have slightly annoying notational conventions H is used here to denote the Hadamard gate but H is also often used to denote a Hamiltonian. It's usually clear from the context. You'll get used to it and it won't bother you after a while.

We generally assume that the quantum computer is initialised in the all zero state $|00...000\rangle$. Then gates are applied to prepare a more interesting state. For example, to prepare a Bell state we can apply a Hadamard and then a CNOT:

$$\text{CNOT}(H \otimes \mathbb{I})|00\rangle = \text{CNOT}\frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right)|0\rangle = |\Phi^+\rangle\,. \tag{6.1}$$

Exercise: How could you prepare the $|\Psi^-\rangle$ Bell state?

Measurements are typically performed in the computational basis. That is, you perform a projective measurement on each qubit in the $\{|0\rangle\langle 0|, |1\rangle\langle 1|\}$ basis. In practise this is done by running the circuit many many times and counting the number of times you obtain the 0 outcome. For example, to measure $|\langle 00|\Phi^+\rangle|^2$ you could prepare the $|\Phi^+\rangle$ state as above and then say

$$|\langle 00|\Phi^+\rangle|^2 = p_{00} \approx \frac{N_{00}}{N} \tag{6.2}$$

where N is the total number of times that the circuit was run and N_{00} is the number of times that both qubits were found to be in the 0 state.

To measure an observable a little more classical post processing is required. For example, to measure $\sigma_z = |0\rangle\langle 0| - |1\rangle\langle 1|$ on the first qubit we have

$$\langle\Phi^+|(\sigma_z \otimes \mathbb{I})|\Phi^+\rangle = (p_{00} + p_{01}) - (p_{10} + p_{11}) \approx \frac{N_{00}}{N} + \frac{N_{01}}{N} - \frac{N_{10}}{N} - \frac{N_{11}}{N}\,. \tag{6.3}$$

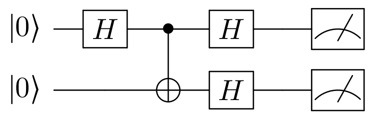
And what about measuring in a basis other than the computational basis? Well in that case you need to first transform into that basis. For example, to measure in the $|++\rangle$ basis where $|+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) = H|0\rangle$ you notice that

$$|\langle ++|\psi\rangle|^2 = |\langle 00|H^\dagger \otimes H^\dagger|\psi = |\langle 00|H \otimes H|\psi\rangle|^2 = |\langle 00|(H \otimes H|\psi\rangle)|^2\,. \tag{6.4}$$

Therefore you can just apply $H \otimes H$ to your state and then measure in the computational basis.

Exercise: How would you measure in the σ_x basis?

Quantum circuits are drawn from left to right (the opposite direction to the order you write matrices). For example, the circuit to prepare the $|\Phi^+\rangle$ state and measure in the $|++\rangle$ basis is given by:



(6.5)

Mathematically, we would write this as $|\langle 00|(H \otimes H)\text{CNOT}(H \otimes \mathbb{I})|00\rangle|^2$.

So far we have not really done anything new. I've essentially just shown you a (time) discretised way of looking at the evolution of quantum systems where time evolutions are broken up into discrete chunks, i.e. gates. All quantum circuits (i.e. all possible unitary evolutions on systems of qubits) can be constructed using sequences of the gates H, S, T, and C_{NOT} gates; however, for arbitrary circuits this can take exponential time. Some algorithms, on the other hand, do not require a complex architecture and are, therefore, very efficient. Let's look at a pedagogical example of one.

6.2 Deutsch's Algorithm

Let us start with Deutsch's algorithm as an example of a quantum algorithm. This algorithm is of historical importance as the first example of a quantum algorithm with a proven exponential advantage. It also can also be used to introduce the notion of *quantum parallelism*. This gives an intuitive notion of where, in part, quantum computers gain their power. However, this intuitive notion should be taken with a pinch of salt as it can be be easily misunderstood.

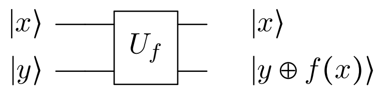
Task: Given a Boolean function $f(x) : \{0,1\} \to \{0,1\}$ we want to determine whether $f(x)$ is constant or balanced, meaning either $f(1) = f(0)$ or $f(1) \neq f(0)$, respectively. Classically, it is necessary to evaluate the function twice to determine this. Deutsch's algorithm allows us to know this characteristic in a single evaluation.

How do we encode this function in a quantum computation? You might hope that you could find a unitary such that

$$|i\rangle \; -\boxed{U}- \; |f(i)\rangle \tag{6.6}$$

However with a little thought we can see that this operation is not reversible and so there is no such unitary. For example, say $f(0) = f(1) = 0$ then we would have $|0\rangle \to |0\rangle$ and $|1\rangle \to |0\rangle$ which clearly isn't unitary.

Instead we need to introduce an ancilla qubit which keeps track of the input. Specifically, we will consider a quantum gate U_f



where $|x\rangle$ and $|y\rangle$ represent one qubit each and $\oplus$ denotes modulo-2 addition. This is a reversible way of implementing the function f in a quantum circuit. The unitary U_f is known as a quantum oracle because it is typically treated as a blackbox that is given to you. However, note that nothing so far is inherently quantum.

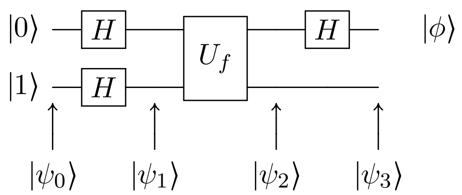
But let's see what happens if you feed in a superposition:

$$|+\rangle|0\rangle = \frac{1}{\sqrt{2}}\left(|00\rangle + |10\rangle\right) \to \frac{1}{\sqrt{2}}\left(|0f(0)\rangle + |1f(1)\rangle\right) \,. \tag{6.7}$$

We have the function evaluated at both of the possible inputs in the superposition. This is known as ***quantum parallelism***, with one oracle call, we have *in some sense* evaluated both outcomes.

But if you measure either qubit you get either $|0f(0)\rangle$ or $|1f(1)\rangle$ with equal probability. So you are back to the classical situation. If we want to make the most of this quantum parallelism we need to be cleverer.

Deutsch's algorithm does this. Consider the circuit:



where H is the Hadamard gate, which sends $|0\rangle \to \frac{|0\rangle+|1\rangle}{\sqrt{2}}$, and $|1\rangle \to \frac{|0\rangle-|1\rangle}{\sqrt{2}}$, $|\psi_0\rangle$, $|\psi_1\rangle$, $|\psi_2\rangle$, $|\psi_3\rangle$ the intermediary states, and $|\phi\rangle$ the final state of the first registry. The final state of the second registry is not presented.

Let us detail the intermediary states. Firstly

$$|\psi_0\rangle = |0\rangle \otimes |1\rangle = |0,1\rangle = |01\rangle \,,$$

and

$$\begin{aligned}
|\psi_1\rangle &= (H \otimes H)\,|\psi_0\rangle = (H \otimes H)\,|0\rangle \otimes |1\rangle \\
&= (H\,|0\rangle) \otimes (H\,|1\rangle) \\
&= \left(\frac{|0\rangle + |1\rangle}{\sqrt{2}}\right) \otimes \left(\frac{|0\rangle - |1\rangle}{\sqrt{2}}\right) \\
&= |+-\rangle\,.
\end{aligned}$$

Before computing $|\psi_2\rangle = U_f\,|\psi_1\rangle$, let us first note that

$$\begin{aligned}
U_f|x-\rangle = U_f\,|x\rangle \otimes \left(\frac{|0\rangle - |1\rangle}{\sqrt{2}}\right) &= |x\rangle \otimes \left(\frac{|f(x)\rangle - |1 \oplus f(x)\rangle}{\sqrt{2}}\right) \\
&= \begin{cases} |x\rangle \otimes \left(\dfrac{|0\rangle - |1\rangle}{\sqrt{2}}\right) & \text{if } f(x) = 0 \\ |x\rangle \otimes \left(\dfrac{|1\rangle - |0\rangle}{\sqrt{2}}\right) & \text{if } f(x) = 1 \end{cases} \\
&= |x\rangle \otimes (-1)^{f(x)} \left(\frac{|0\rangle - |1\rangle}{\sqrt{2}}\right) \\
&= (-1)^{f(x)}|x-\rangle\,.
\end{aligned}$$

This identity will make computing the action of the Deutsch circuit much simpler.

Let's now compute $|\psi_2\rangle$. From the following relation,

$$\begin{aligned}
|\psi_2\rangle = U_f\,|\psi_1\rangle = U_f\,|+-\rangle &= U_f\left(\frac{|0-\rangle + |1-\rangle}{\sqrt{2}}\right) \\
&= \left(\frac{(-1)^{f(0)}\,|0-\rangle + (-1)^{f(1)}\,|1-\rangle}{\sqrt{2}}\right) \\
&= \left(\frac{(-1)^{f(0)}\,|0\rangle + (-1)^{f(1)}\,|1\rangle}{\sqrt{2}}\right) \otimes |-\rangle \\
&= \begin{cases} (-1)^{f(0)} \left(\dfrac{|0\rangle + |1\rangle}{\sqrt{2}}\right) \otimes \left(\dfrac{|0\rangle - |1\rangle}{\sqrt{2}}\right) & \text{if } f(0) = f(1) \\ (-1)^{f(0)} \left(\dfrac{|0\rangle - |1\rangle}{\sqrt{2}}\right) \otimes \left(\dfrac{|0\rangle - |1\rangle}{\sqrt{2}}\right) & \text{if } f(0) \neq f(1) \end{cases} \\
&= \begin{cases} (-1)^{f(0)}|+-\rangle & \text{if } f(0) = f(1) \\ (-1)^{f(0)}|--\rangle & \text{if } f(0) \neq f(1) \end{cases}
\end{aligned}$$

Now we see that whether the function is odd or even is directly encoded into the state of the first qubit. All that remains is to read it out. If we measured in the computational basis this would fail because we would get 0 or 1 with equal probability. We need to instead rotate into the X basis. This is done by applying a Hadamard gate H. On doing so we get:

$$\begin{aligned}|\psi_3\rangle &= (H \otimes \mathbf{1})|\psi_2\rangle \\ &= \begin{cases}(-1)^{f(0)}|0-\rangle & \text{if } f(0) = f(1) \\ (-1)^{f(0)}|1-\rangle & \text{if } f(0) \neq f(1)\end{cases} \\ &= (-1)^{f(0)}|f(0) \oplus f(1)\rangle \otimes |-\rangle\end{aligned}$$

We only need then to measure the first qubit in the computational basis $\{|0\rangle, |1\rangle\}$. The result of such a measurement will tell us with certainty if $f(x)$ is constant or balanced.

We see here that there are two ingredients for quantum advantage. Quantum parallelism and a clever manipulation of interference. This gives a hint as to where some of the power of quantum computing comes from. But it is important to be aware that there are many caveats. And exactly what gives quantum computing its power is something still debated.

Note also that here we only saw factor of 2 improvement. It is possible to generalise this problem to a function:

$$f : \{0,1\}^n \to \{0,1\}$$

that takes n-bit binary values as input and produces either a 0 or a 1 as output for each such value. We are promised that the function is either *constant* (0 on all inputs or 1 on all inputs) or *balanced* (1 for exactly half of the inputs and 0 for the other half). The goal is to determine if f is constant or balanced. Classically solving this problem requires $2^{n-1} + 1$ oracle calls. But using a quantum algorithm (the Deutsch-Jozsa algorithm the problem can be solved with only one oracle call. Thus a quantum computer can seemingly achieve an exponential speed up. To read more about this algorithm go to Nielson and Chuang (or any other quantum computing textbook.

If this all seems a little abstract and pointless. Don't worry the Deutsch algorithm is rather pointless. It also relies on access to an oracle and it's far from clear how one could ever have one of those and not actually know the function itself. This example is largely for pedagogical value. We will now move on to discussing briefly some potentially more useful applications of quantum computing.

6.3 Quantum simulation

The simplest motivation for quantum computing, first highlighted by Feynman in the 1980s, is to simulate quantum systems.

Imagine trying to numerically simulate n-qubits. That is you have an n qubit state and you want to compute its evolution under e^{-iHt}. If H is something messy and complicated (as for most real physical systems) you can not do this 'by hand' and so instead you want to do it numerically. But now a n qubit state is 2^n dimensional, i.e. its basis is $|\tilde{0}\rangle = |00...00\rangle$, $|\tilde{1}\rangle = |00...01\rangle$, $|\tilde{2}\rangle = |00...10\rangle$ all the way to $|\tilde{2^n}\rangle = |11...11\rangle$. Thus we need to store an exponentially large vector. To compute its evolution we then need to multiply by e^{-iHt}, which is a 2^n by 2^n dimensional unitary. Storing this again requires exponential memory. And performing the matrix multiplication will take exponential time.

More generally, consider a quantum system of N particles characterized by the wave function $\Psi(r_1, \cdots, r_N, t)$ and the evolution equation [4]:

$$i\frac{\partial\Psi}{\partial t} = H\Psi$$

For the numerical simulation of this system, it's necessary to discretize time as well as space. Let's assume a spatial grid of M cells. For $3N$ coordinates, we have $(M)^{3N}$ elements. So, the matrix H has a size of $(M)^{3N} \times (M)^{3N}$. Thus we need exponential memory just to store the matrix for the Hamiltonian... and then we need to think about manipulating (e.g. exponentiating it).

Feynman sees this limitation as an opportunity, through the following reflection: a classical computer takes time $T = \mathcal{O}(\Delta t \cdot \mathrm{const}^N)$ to simulate this system, while nature takes time $T = \mathcal{O}(\Delta t)$! Nature can solve an intractable problem for classical computers with zero complexity. Or in the more poetic but unbelievably over quoted words of Feynmann:

"*Nature isn't classical, dammit, and if you want to make a simulation of nature, you'd better make it quantum mechanical...*"

To simulate a quantum system on a quantum computer you 'just' need to be able to implement (or approximately implement) the unitary

$$U = e^{-iHt} \tag{6.8}$$

on your quantum computer. That is, you need to be able to break it down into a series of basic gates. By now there have been many approaches established to do this. If you are interested in learning more one of the standard approaches is Trotterization based simulation where the total evolution is broken down into a series of short time steps for which you can assume terms in the Hamiltonian approximately commute. If you are interested to learn more about this technique (and others) I'd recommend Giuseppe Carleo's course on Computational Quantum Physics.

The main point I want to stress in this brief section, partially because this was not made clear enough to me when I first learnt about quantum computing, is that one of the main arguments for building quantum computers is to be able to better simulate quantum systems. This would make the lives of quantum chemists, material scientists, high energy physicists... all sorts of folk much easier.

6.4 Variational quantum algorithms

Variational quantum algorithms are a very popular [5] form of quantum algorithm being investigated currently. This is part of my motivation to briefly introducing them to you now - if you stay in quantum computing you are very likely to encounter them. But I also want to introduce them as a stepping stone to introducing quantum machine learning, which in turn I want to introduce to provide a practical example use of groups and representations. Realistically probably more of you will end up working in machine learning than in physics so I want to (if I have time!) showcase how groups and reps can be useful in that context.

A good introduction to VQAs is provided here. This is much much more than you need for this course but I share in case it is of interest. And because I am about to shamelessly [6] quote

[4] As should be clear from the context H is back to being a Hamiltonian here.

[5] A quick search on google scholar for "variational quantum" throws up 12800 hits.

[6] I'm friends with the first author, it's ok, maybe. Do as I say not as I do.

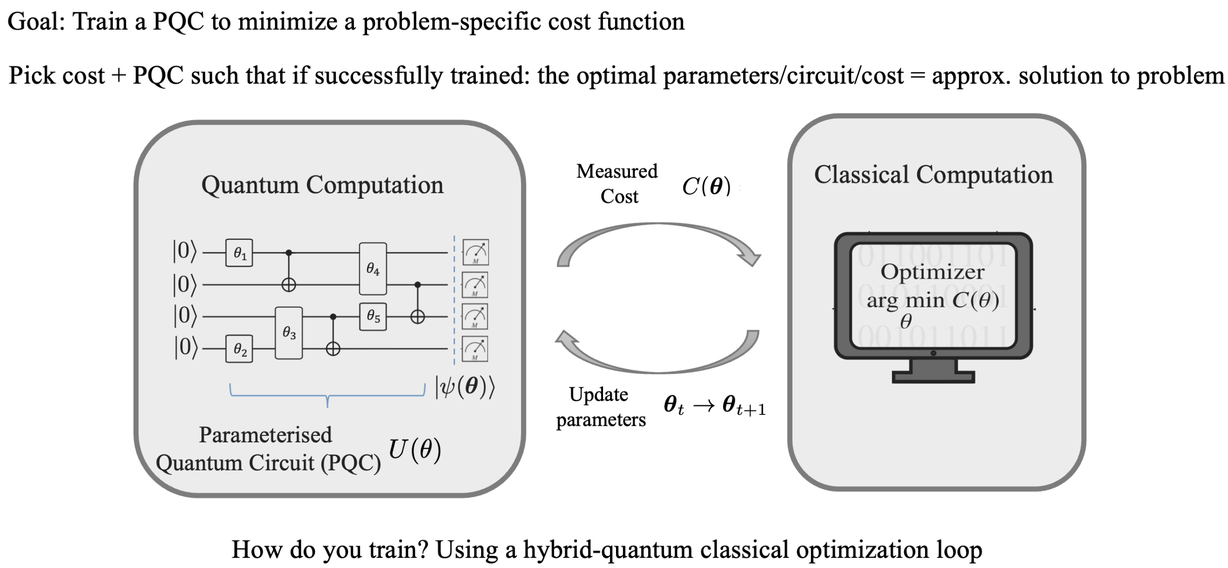


Figure 6.1: A hybrid quantum classical optimization loop is used to optimize a variational .

text from there now:

One of the main advantages of VQAs is that they provide a general framework that can be used to solve a variety of problems. Although this versatility translates into different algorithmic structures with different levels of complexity, there are basic elements that most (if not all) VQAs have in common.

Let us start by considering a task one wishes to solve. This implies having access to a description of the problem, and also possibly to a set of training data. The first step to developing a VQA is to define a cost (or loss) function C which encodes the solution to the problem. One then proposes an ansatz, that is, a quantum operation depending on a set of continuous or discrete parameters θ[7] that can be optimized (see below for a more in-depth discussion of ansatzes). This ansatz is then trained in a hybrid quantum-classical loop to solve the optimization task.

$$\theta^* = \arg\min_{\theta} C(\theta) \tag{6.9}$$

The trademark of VQAs is that they use a quantum computer to estimate the cost function $C(\theta)$ (or its gradient) while leveraging the power of classical optimizers to train the parameters θ.

This hybrid-quantum classical optimisation loop is sketched in Fig. 6.1.

Crucial to any variational quantum algorithm is your choice in cost function. The idea is to pick your cost such that by minimising the cost you solve whatever problem it is you are trying to solve. Similar to classical machine learning, the cost function maps values of the trainable parameters (i.e. the vector $\overline{\theta} = (\theta_0, \theta_1, \theta_2, ..., \theta_L)$ to real numbers. The simplest choice in quantum cost function one can consider is simply the expectation value of some measurement operator in some parameterized state:

$$C(\theta) = \mathrm{Tr}[OU(\theta)\rho U^\dagger(\theta)] \tag{6.10}$$

[7]Please note that all of these θs (i.e. any θ without a subscript) should be vectors. LaTeX is being stroppy and doesn't want to make them bold for me right now. I'll sort this in an updated version of these notes.

Here ρ is some initial state, $U(\theta)$ is a parameterized quantum circuit (more on this in a second), and O is some Hermitian observable. Note that this cost can be read as either quantifying the expectation of some observable O given a parameterized state $\rho(\theta) := U(\theta)\rho U^\dagger(\theta)$ or the expectation of some parameterized observable $O(\theta) = U^\dagger(\theta) O U(\theta)$ given some fixed input state ρ, that is:

$$C(\theta) = \mathrm{Tr}[O\rho(\theta)] = \mathrm{Tr}[\rho O(\theta)] \, . \tag{6.11}$$

Thus a VQA can broadly be read as either trying to find the 'best state' to solve your problem, or 'best observable' to solve your problem.

The final ingredient is the parameterized quantum circuit (PQC). As the name sounds this is a quantum circuit, i.e., some arrangement of quantum gates, but with some of those angles parameterized. This can generically be represented as the product of m simpler parameterized unitaries, interspersed with non-parameterized unitaries:

$$U(\theta) = \prod_m e^{-i\theta_m P_m} W_m \, . \tag{6.12}$$

Here W_m are unparametrized unitaries (for a simple choice consider a ladder of CNOTs) and P_m are Pauli operators. For example, if each P_M is a single qubit Pauli then a term of the form

$$e^{-i\theta_m P_m} \tag{6.13}$$

will induce a parameterized rotation about axis P_m on the Bloch sphere. I'll sketch an example of this on the board in the lecture.

The paradigmatic example of a variational quantum algorithm is the variational quantum eigensolver. The goal here is to learn the ground state of a given Hamiltonian H. The observable used in the cost in this case is simply H and we consider a pure input state $\rho = |0\rangle\langle 0|$. Thus the cost simplifies to:

$$C(\theta) = \langle \psi(\theta)|H|\psi(\theta)\rangle = \langle 0|U(\theta)^\dagger H U(\theta)|0\rangle \, . \tag{6.14}$$

The state that minimizes this cost $|\psi(\theta^*)\rangle$ is the state that has the lowest average energy, i.e. is the ground state: $|\psi(\theta^*)\rangle = |E_{\text{ground}}\rangle$ And the energy of this state corresponds to the ground state energy: $C(\theta^*) = \langle \psi(\theta^*)|H|\psi(\theta^*)\rangle = E_{\text{ground}}$.

This is just one example of a variational quantum algorithm. There are many many more. I'll now move onto discussing a variational quantum algorithm that can be used for classification (i.e. has more of a machine learning flavour).

6.5 Quantum Machine Learning

Let's consider a binary classification task. In a binary classification task, we have a dataset $\mathcal{D} = \{x_i, y_i\}_{i=1}^M$ with data points $x_i \in \mathbb{R}$ and labels $y_i \in \{0, 1\}$ and we want to learn a strategy for distinguishing x's corresponding to $y = 0$ labels and x's corresponding to $y = 1$ labels.

More concretely, let's suppose I want to classify the following data set [8]: But I am a human and so I am lazy and so I want to draw a line, i.e., a classifying plane, and I want to assign a label to everything that is to the left of the line and a label to everything that is to the right of the line.

[8] I have borrowed this example from Marco Cerezo.

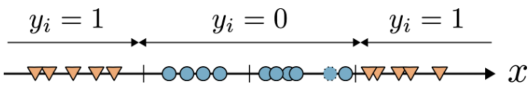


Figure 6.2: A simple classification problem.

Now obviously this isn't possible with the data in its current form. Let's first see how this could be done using (simple) **classical machine learning**.

The first classical strategy we can consider is to map the data to a higher dimensional space. A simple mapping in this case is simply to send $x \to x^2$. Now the data is linearly separable:

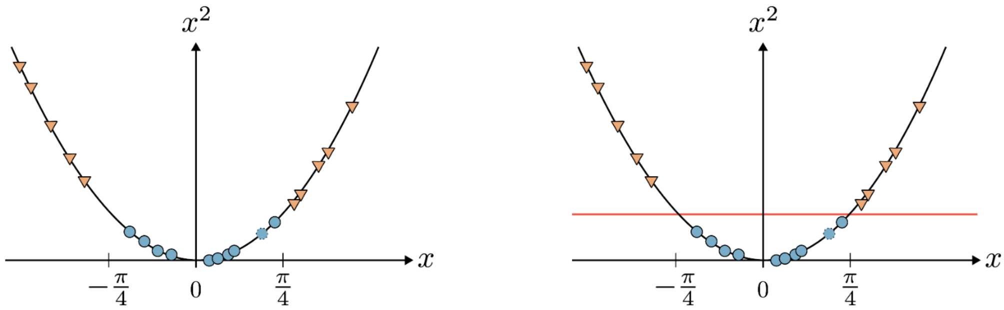


Figure 6.3: Classification via mapping to a higher dimensional space.

A second classical approach would be to train a neural networks to process the data and learn a classifying function. A neural network is just a composition of neurons, where the neurons are simply functions that take an input, and spit out an output. Let's consider a very simple neural network with one input layer that takes x, two hidden neurons, and one output neuron: The neurons just take their input, multiply by a weight, add a bias, and have some activation

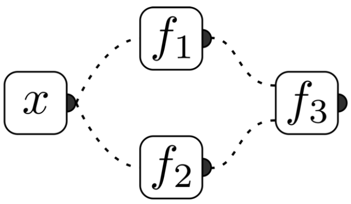


Figure 6.4: Simple neural network.

function which I'll take to be the sigmoid function. Concretely, I'll suppose that each of neurons output:

$$\begin{aligned} f_1(x) &= \text{sigmoid}(w_1 x + b_1) \\ f_2(x) &= \text{sigmoid}(w_2 x + b_2) \\ f_3(x_1, x_2) &= \text{sigmoid}(w_{31} x_1 + w_{32} x_2 + b_3) \end{aligned} \tag{6.15}$$

where the w_i and b_i are trainable parameters, x, x_1, x_2 are the inputs to the neurons and $\text{sigmoid}(Z) = \frac{1}{1+e^{-z}}$. The output of the neural network is the output of the function f_3, i.e. a single real number.

The aim is to train the weights and biases of neural network, using data from our training set, so that the neural network outputs the correct label. More concretely, let's write the function implemented by the neural network as $f_{\mathbf{w},\mathbf{b}}(x)$. We train our cost by minimising:

$$C(\mathbf{w},\mathbf{b}) = \sum_i (f_{\mathbf{w},\mathbf{b}}(x_i) - y_i)^2\,. \tag{6.16}$$

where the sum is over data in the dataset $\mathcal{D}$. We can try this and it works, we can indeed classify the data this way:

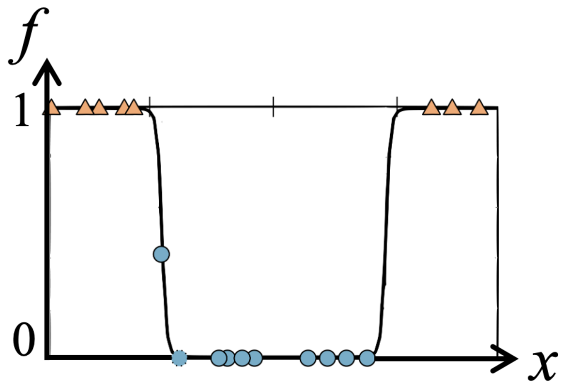


Figure 6.5: Classification via a classical neural network.

Ok, enough of the classical case. How could this be done using **quantum machine learning**? A parameterized quantum circuit (which in this context is often called a *quantum neural network*) uses a combination of the two methods described above to classify data. That is, a PQC can both map the input data to a higher dimension and be used to process that data.

Let us consider performing this classification task on a quantum computer using a single qubit. The first step will be to embed the data into a quantum state. This can be done using a single rotation around the y axis where the rotation angle is given the input x_i. Let us sketch the effect of this:

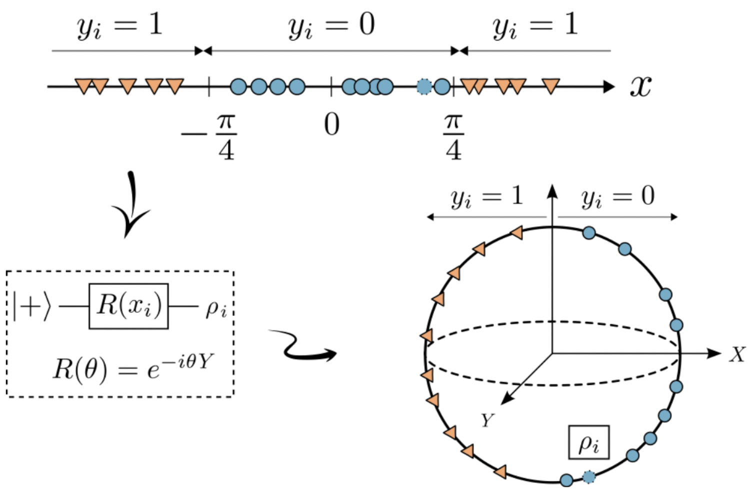


Figure 6.6: Encoding data in a single qubit

Notice the similarities between this case and the classical mapping to a higher dimensional space shown in Fig. 6.3. The data which previously was not linearly separable now looks suspiciously linearly separable.

The final step is to learn a measurement that can indeed perform the classification. That is, given an encoded input state ρ_x we want to learn a measurement $M(\theta)$ we can perform on ρ_x that can spit out the correct $y = 0$ or $y = 1$ label. (For this easy example we can just read it off from the figure above- the optimal measurement will be a measurement in the X basis- but it will not always be this easy so let's pretend we can't read it off). We can propose a trainable classifier of the form:

$$f_\theta(x) := \mathrm{Round}\left(\mathrm{Tr}[\rho_x M(\theta)]\right) , \tag{6.17}$$

where $M(\theta) = U^\dagger(\theta)|0\rangle\langle 0|U(\theta)$ and train using a cost of the form

$$C(\theta) = \sum_i (f_\theta(x_i) - y_i)^2 . \tag{6.18}$$

On training this we do indeed find that the we learn the optimal classifying where $M = |+\rangle\langle +|$. Here's a plot from the training showing that it does indeed work:

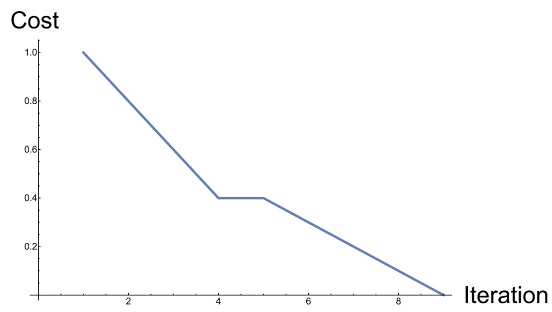


Figure 6.7: Training a single qubit QNN.

This was a very simple example of how quantum circuits can be used for machine learning. The paradigm is highly flexible, though its power and limitations are still very much up for debate. As I said previously, if you want to know more this is good place to start.

Chapter 7

Symmetry in quantum mechanics

7.1 Introduction

These notes are driven by the pedagogical philosophy that most people learn best by examples and intuition. Therefore, throughout these notes I try as hard as I can to provide examples and more informal handwavey explanations of the key ideas wherever possible. In places I have sacrificed some formality to do so. I have also for the sake of time relegated some of the longer proofs to the appendices. If you are interested in a more formal presentation of this material I have uploaded to moodle Vincenzo Savona's old notes (in French and English). However, I hope my notes will prove helpful to those of you who also like examples and an attempt at more wordy explanations.

7.1.1 Motivational example on spatial translations

By way of introduction let's start with a simple example considering spatial translations that I have borrowed from Terry Rudolph. Suppose I asked you to write down a wavefunction $\psi(x)$ that is invariant under arbitrary translations in x, i.e. $x \to x + a$ for any a. What could you write down?

Intuitively if it's anything other than constant in x then the function will not be spatially invariant, i.e. we've got to have $\psi(x) = \text{constant}$. In Terry's words - *It is questionable whether this is valid - is it normalizable for example? But imagine we plough ahead like good physicists and ignore the mathematical difficulties.* If we Fourier transform this wavefunction then we get that this wavefunction can be written in the momentum basis as $\phi(p) = \delta(p)$ (the Fourier transform of the constant function is a delta function).

But is this the only function that is invariant under spatial translations? What if we instead consider a function of the form $\psi(x) = e^{ipx}$? Then we see that translating $x \to x + a$ produces only an extra "overall phase" of e^{ipa}. This is a global phase and so doesn't change anything physical about the state. That is, the state is (up to a non-physical global phase) also invariant under translations. If we again Fourier transform to the momentum representation we now have $\psi(x) = e^{ipx}$ is $\phi(p) = \delta(p - p')$, so this is a state of fixed definite momentum p'. That is, momentum is conserved in this translationally invariant state.

In Terry's words again we learn two things from this example: *(i) that we should only expect a small subset of the possible quantum states to obey a particular symmetry, and (ii) that there can be an intimate connection between a particular observable (momentum) and that symmetry.*

Exercise: show that the momentum operator $\hat{p}$ is the generator of spatial translations, by *which (for now* [1]*) we mean:*

$$e^{-i\hat{p}b}\psi(x) = \psi(x+b). \tag{1}$$

Now imagine we have prepared one of these translationally invariant states, e.g. a momentum eigenstate. Under what Hamiltonian evolutions will it remain translationally invariant/a momentum eigenstate? Intuitively we need any potential $V(x)$ to also be translationally invariant, otherwise this will break the initial translational symmetry. This means the only potential Hamiltonian is the free particle Hamiltonian $H = \frac{1}{2m}\hat{p}^2$. Or, more concretely, we require that

$$[e^{-i\hat{p}b}, \hat{H}] = 0. \tag{2}$$

which will be true for any Hamiltonian such that $[\hat{p}, \hat{H}] = 0$. Thus we see that the property of translational symmetry is associated with 'conservation of momentum'.

A similar story could be told about the relationship between rotational invariance and angular momentum. And both of these cases are symptomatic of a much deeper story about the intimate connection between conservation laws and stuff that commutes with a Hamiltonian and symmetries. This can be made precise and of sweeping generality in Noether's theorem. But let's start with the basics and pin down a more general mathematical formalism to discuss symmetries.

7.1.2 Introduction to groups

A symmetry describes some property of a system, i.e. some function f or of some dataset $\mathbb{R}$, which is left unchanged under some transformation. As we are, for the purpose of this course, predominantly interested in quantum systems, let's suppose that the transformation refers to a *unitary evolution*[2] applied to the quantum state, i.e., to a map $\rho \to U\rho U^\dagger$ for some U. Now crucially, such symmetry transformations form *a group*.

Proposition 7.1.1. *Let G be the set of all unitary symmetry transformations, such that for any $U \in G$, the map $\rho \to U\rho U^\dagger$ leaves some property of ρ unchanged. Then, G, equipped with multiplication, forms a group.*

What is a *group*?

Definition 7.1.2. A group is a set equipped with an operation that combines any two elements to form a third element while being associative as well as having an identity element and inverse elements.

Formally, one can write a set G equipped with the operation "$*$" is a group if one has:

- G is closed under the operation $*$. That is, if $a \in G$ and $b \in G$ then $a * b \in G$.
- Associativity: $\forall a, b, c \in G$, one has $(a * b) * c = a * (b * c)$.
- An identity element: There exists an element $e \in G$ such that $e * a = a \ \forall a \in G$. Such an element is unique and is called the identity of the group.
- Inverse element: $\forall a \in G$, it exists $b \in G$ such that $b * a = a * b = e$. We then say that $b = a^{-1}$. For each e the element a^{-1} is unique and is called the inverse of a.

[1] We will define the term generator more formally when we define Lie Algebras.

[2] We will encounter and work with symmetry representations that are ostensibly not unitary. However, a wide class of representations are equivalent to unitary ones. In particular, Wigner's theorem guarantees that all symmetry transformations of quantum states preserving inner products are either unitary or antiunitary, and often antiunitary transformations are "unitary and complex conjugation".

How can we see that any unitary that leaves a property invariant forms a group with $*$ matrix multiplication (i.e. that Proposition 7.1.1 is true)? With a little thought we can see that each of the defining properties of a group are satisfied.

- Closure: Given any two unitaries U and V in G, the unitary $V * U$ obtained by multiplying V and U is also a symmetry transformation. This follows from the fact that concatenating two property-preserving transformations $\rho \to U\rho U^\dagger \to V * U\rho U^\dagger * V^\dagger$ constitutes in itself a property-preserving transformation.
- Associativity: for any unitaries U, V, W we have $U(VW) = (UV)W$.
- Identity element: Clearly the identity matrix I leaves any property of a state unchanged and for any unitary we have $IU = U$ and so I is indeed the identity element e.
- Inverse: For each U in G, there exists an element $U^\dagger$ in G such that $U * U^\dagger = U^\dagger * U = I$, where I is the identity matrix, and $U^\dagger$ is the inverse (conjugate transpose) of U because if U conserves some property, then U^{-1} also conserves that property.

In broad terms *groups* encode abstract symmetries, and *representations* describe concrete realisations of those symmetries in physical systems. In most maths courses people learn about groups first before moving onto representations later. However, in practise, in everyday physics we often identify symmetries at the level of the representation and then "abstractify" them: i.e. connect a familiar physical symmetry with some familiar abstract mathematical group.

To quote Representation Theory for Geometric Quantum Machine Learning: *"The main utility of this abstractification procedure is that groups as mathematical objects have been thoroughly studied since the early 19th century, and a wealth of information is readily available for scores of them. Moreover, in the eyes of physics, the list of abstract groups is surprisingly short, thanks in large part to classification programs for finite groups and semisimple Lie groups—and nature's seeming preferential treatment of these groups—this means that identification is direct in many cases."* That is, if you have a physics (or perhaps even a classical machine learning) problem and can identify the relevant group - odds are some long dead mathematician has already half solved your problem and so you can save yourself a lot of work.

In broad terms a representation is a map from the elements of a group to a set of unitaries[3] such that the unitaries obey the same properties under composition as the original group. We will define this more formally later but I just wanted to mention it informally now because I think it helps to understand why we care about groups in the first place- the key point being often in practise we will identify the representation first and then abstractify to find the underlying group and then plug in centuries of maths to help us understand it better.

7.1.3 Finite group examples

Groups can be either finite or continuous. Let's consider some examples of finite groups first.

Definition 7.1.3 (Finite group)**.** A group that contains a finite number of element is called a finite group. The number of element is called the *order* of the group.

One way to uniquely identify a group is via its Cayley table. Named after the 19th century British mathematician Arthur Cayley, a Cayley table describes the structure of a finite group by arranging all the possible products of all the group's elements in a square table reminiscent of an addition or multiplication table. Many properties of a group can be discovered from its Cayley table.

[3]Representations need not strictly be unitary but essentially all the ones we'll care about here will be.

Order 1 group. The only group with only one element is the trivial group containing just the identity element, e.g. $G = e$. Its Cayley table can be written as:

$$\begin{array}{c|c} * & e \\ \hline e & e \end{array} \tag{7.1}$$

A possible representation of this group is $e \to I$.

Order 2 group. The unique Cayley table for a group with only two elements is the group where the only non-identity element is its own inverse element, e.g. $G = e, a$ such that $aa^{-1} = aa = e$, i.e.

$$\begin{array}{c|cc} * & e & a \\ \hline e & e & a \\ a & a & e \end{array} \tag{7.2}$$

One possible group with this Cayley table is $G = \{1, -1\}$ with $*$ standard scalar multiplication. (In this case, the map $e \to 1$ and $a \to -1$ is a representation of the group)

Other examples include the groups composed of $G = \{I, X\}$, $G = \{I, Z\}$ and $G = \{I, \mathrm{SWAP}\}$ with $*$ matrix multiplication. (In this case, the maps $e \to I$, $a \to X$ and $e \to I$, $a \to Z$ and $e \to I$, $a \to \mathrm{SWAP}$ are representations of the group).

Another possible group with the same Cayley table is the parity group that contains the "transformation in the mirror" that turns x into $-x$. Let us define the operator $\hat{P}$ such that $\hat{P}f(x) = \hat{P}f(-x)$. Given $\hat{P}\hat{P} = 1$, we see that the set of transformation $\{1, \hat{P}\}$ form a group.

All of these groups are isomorphic (share the same Cayley table) to the $\mathbb{Z}_2$ group (cyclic group on 2 elements). The Cayley table captures the fundamental symmetry but it can manifest in different ways.

Order 3 group. The unique (it might not be obvious now that it is unique - we will come back to this in a bit) Cayley table for a group with only three elements is the $\mathbb{Z}_3$ group (cyclic group with three elements):

$$\begin{array}{c|ccc} * & e & a & b \\ \hline e & e & a & b \\ a & a & b & e \\ b & b & e & a \end{array} \tag{7.3}$$

An example of such group is the set of 2D rotations that leave a triangle invariant. Or the 3rd roots of unity in the complex plane $a_j = e^{i2\pi\frac{j}{3}}$ equipped with multiplication.

Order 4 groups. Again we can consider the cyclic group $\mathbb{Z}_4$

$$\begin{array}{c|cccc} * & e & a & b & c \\ \hline e & e & a & b & c \\ a & a & b & c & e \\ b & b & c & e & a \\ c & c & e & a & b \end{array} \tag{7.4}$$

An example of such group is the set of 2D rotations that leave a square invariant. Or the 4th roots of unity in the complex plane.

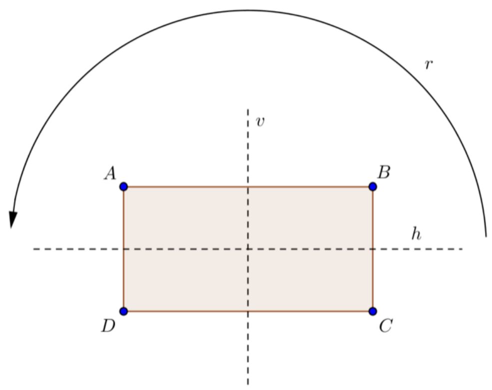


Figure 7.1: Diagram of the symmetry group of a rectangle (dihedral group R_2): (Wiki page on the Dihedral group).)

But 4th order is also the smallest order that is not unique. That is, there is another possible Cayley table for a group of four elements that is not isomorphic (i.e. the same up to relabeling) as the Cayley table above:

$$\begin{array}{c|cccc} * & e & a & b & c \\ \hline e & e & a & b & c \\ a & a & e & c & b \\ b & b & c & e & a \\ c & c & b & a & e \end{array} \tag{7.5}$$

Note that here each element is its own inverse but there are cyclic transformations between a, b and c. An example of such a group would be the symmetries of a rectangle as sketched in Fig. 7.1. The group elements are identity e, rotation r (in either direction) by π and reflections h and v about the horizontal and vertical axes respectively.

Order 6 groups. Again we can consider the cyclic group $\mathbb{Z}_6$. Alternatively we can have:

$$\begin{array}{c|cccccc} * & e & a & a^2 & b & c & d \\ \hline e & e & a & a^2 & b & c & d \\ a & a & a^2 & e & c & d & b \\ a^2 & a^2 & e & a & d & b & c \\ b & b & d & c & e & a^2 & a \\ c & c & b & d & a & e & a^2 \\ d & d & c & b & a^2 & a & e \end{array} \tag{7.6}$$

This is called the C3v group.. This is the symmetry group of a triangle as shown in Fig. 7.2. There are 6 possible transformations that leave the triangle invariant:

- The identity e which leaves all coordinates unchanged.
- The proper rotation c_+ by an angle of $2\pi/3$ in the positive trigonometric sense (i. e. counter-clockwise). And the clockwise version c_-.
- Reflection along each axis (there are three of them).

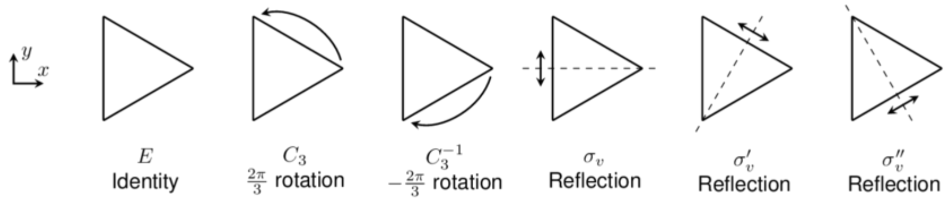


Figure 7.2: Diagram of the symmetry group of a triangle (C3v). Note that I used the notation $c_+ = C_3$ and $c_- = c_-$ to denote the rotations but this image uses C_3 and c_-. I took this image from (Fundamental properties of 2D excitons bound to single stacking faults in GaAs).)

See Fig. 7.2 for a sketch of this. The C3v also captures the symmetry of the Ammonia molecule, NH3. There will be a question on the problem sheet this week on this. This will be one of our favorite example groups so its worth becoming very familiar with it.

Other important (larger) finite groups include:

The cyclic group $\mathbb{Z}_n$. For completeness, of course we can also consider the cyclic group of n objects $\mathbb{Z}_n$

$$\begin{array}{c|cccccc} * & e & a_1 & a_2 & \dots & a_{n-1} \\ \hline e & e & a_1 & a_2 & \dots & a_{n-1} \\ a_1 & a_1 & a_2 & a_3 & \dots & e \\ a_2 & a_2 & a_3 & a_4 & \dots & a_1 \\ \vdots & & & & & \\ a_{n-1} & a_{n-1} & e & a_1 & \dots & a_{n-2} \end{array} \tag{7.7}$$

Examples of such groups include the set of 2D rotations that leave a regular n-sided polygon invariant and the nth roots of unity $a_j = e^{i2\pi \frac{j}{n}}$ in the complex plane.

Symmetric permutation group S_n. The group is composed of the group of all possible permutations of n object with the group operation the composition of functions.

As there are $n!$ such permutations operations the order of the symmetric group is $n!$

For example, $S_3 = \{I, \mathrm{SWAP}_{12}, \mathrm{SWAP}_{13}, \mathrm{SWAP}_{23}, \mathrm{CYCLE}_{123}, \mathrm{CYCLE}_{321}\}$. (What is the CAYLEY table for this group? [4])

This is a very important group in quantum physics as (as we saw earlier) it is the symmetry group of systems of indistinguishable particles.

7.1.4 Continuous group examples

A non-finite group is a continuous group. Of particular importance are *Lie* groups.

Definition 7.1.4 (Lie group)**.** Informally, a Lie group is a continuous group that depends *analytically* on some continuous parameters λ.

[4] Hint we have already seen that there are only two possible tables for an order 6 group

Note that not all infinite groups are Lie groups! The set of all rational numbers equipped with addition is infinite (but countable), but it is not a Lie group.

We list some important examples of Lie groups below.

Real d-dimensional rotations $SO(d)$. A classic example of a Lie group is the group of all rotation matrices (i.e. orthogonal matrices with determinant 1) for real d dimensional rotation vectors. An orthogonal matrix is the real analogue of a unitary matrix and is defined by the properties $\Re[M] = M$ and $MM^T = M^T M = I$. For an orthogonal matrix to be a rotation matrix we also require that $det(M) = 1$.

For example, the elements of the group $SO(2)$ (i.e. rotation matrices in $2D$) can be written as

$$M(\phi) = \begin{bmatrix} \cos(\varphi) & -\sin(\varphi) \\ \sin(\varphi) & \cos(\varphi) \end{bmatrix}. \tag{7.8}$$

Another commonly encountered case is $SO(3)$ which corresponds to all rotations in $3D$.

The orthogonal group $O(d)$. Another example of a continuous group is $O(d)$ which is simply the group of orthogonal matrices (i.e. without the restriction that the determinant of the matrices equals 1). Orthogonal matrices preserve the inner product between real vectors $\langle x'|y'\rangle = (\langle x|O^T)(O|y\rangle) = \langle x|O^T O|y\rangle = \langle x|y\rangle$. They thus correspond to rotations and reflections.

Note that the determinant of any orthogonal matrix is +1 or −1. This follows from $1 = \det(I) = \det(M^T M) = \det(M^T)\det(M) = (\det(M))^2$. Orthogonal matrices with a -1 determinant can implement reflections, e.g.

$$M = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \tag{7.9}$$

performs a reflection of the vector (x, y) in the y-plane.

The unitary group $U(d)$. $U(d)$ is the group of $d \times d$ dimensional unitary matrices. This is the group of matrices that preserve the length/inner product of quantum states.

For example, $U(1)$ can be represented just as the unit circle in the complex plane $[e^{i\phi}]$. Or it can be represented as a rotation around any single axis on the Bloch sphere, e.g. $[R_z(\phi)]$ where $R_z(\phi) = e^{-i\phi Z}$.

Similarly, $U(2)$ represents all 2-dimensional unitaries, that is all unitaries on a single qubit. We recall that any single qubit unitary can be written as

$$R(\boldsymbol{n}, \theta, \phi) = e^{-i(\phi I + \theta \boldsymbol{n}.\boldsymbol{\sigma})} \tag{7.10}$$

where we stress that for full generality we need to include the global phase term generated by ϕI. However, this global phase is unphysical. This motivates the consideration of instead the special unitary group.

The special unitary group $SU(d)$. $SU(d)$ corresponds to the group of unitary matrices with determinant 1. The restriction to determinant 1 effectively fixes the arbitrary global phase. To see this note that multiplying a unitary matrix by a phase matrix $e^{-i\phi}I$ manifests as a change in the phase of its determinant as $\det(e^{-i\phi}IM) = \det(e^{-i\phi}I)\det(M) = e^{-id\phi}\det(M)$.

For example $SU(2)$ corresponds to the group of unitary rotations to a single qubit that can be written as

$$R(\boldsymbol{n},\theta) = e^{-i\theta \boldsymbol{n}.\boldsymbol{\sigma}} . \tag{7.11}$$

Recall that this can be represented as the set of rotations of the Bloch vector of a state on the Bloch sphere. This would seem to be *in some sense* equivalent to the group $SO(3)$, i.e. the group of real rotations in 3D. Indeed the groups $SU(2)$ and $SO(3)$ are very closely related - more on this in a bit.

7.2 Basic definitions and properties of groups

Now that you're equipped with a whole zoo of examples let's go back to looking at the basic mathematical structure of groups and some of their most important properties.

Definition 7.2.1 (Abelian and non-Abelian groups)**.** : If $a * b = b * a \ \forall a, b \in G$, the group G is said to be Abelian. Otherwise it is called a non-Abelian group. These groups are also called commutative and non-commutative.

For example, $U(1)$ is Abelian (phases commute) but $U(2)$ is not (arbitrary unitaries do not commute). As we will see later, whether or not a group is Abelian effects some of their most fundamental properties. (In particular, Abelian groups tend to be much simpler to study).

Another very important concept is that of a subgroup.

Definition 7.2.2 (Subgroup)**.** A subset H of the group G is a subgroup of G if and only if it is nonempty and itself forms a group.

The closure conditions mean the following: Whenever a and b are in H, then $a * b$ and a^{-1} are also in H. These two conditions can be combined (*exercise: show this!*) into one equivalent condition: whenever a and b are in H, then $a * b^{-1}$ is also in H. The identity of a subgroup is the identity of the group: if G is a group with identity e_G, and H is a subgroup of G with identity e_H, then $e_H = e_G$.

Definition 7.2.3 (Proper Subgroup)**.** We call a subgroup of G which is neither the identity nor G itself a *proper* subgroup.

A fundamental result in the theory of finite groups is Lagrange theorem:

Theorem 7.2.4 (Lagrange)**.** *Let G be a finite group and H a subgroup of G, then the order of H (i.e. the number of its elements) divides the order of G.*

We prove this theorem in sec.7.14.1.

It is easy to see that this implies in particular that if the order of a group is prime then there is only one possible group (i.e. one unique Cayley table) for that group. To see this note that if the order n of a finite group G is a prime, then it has no divisors, and so no subgroups. The only group with no proper subgroups is the cyclic one Z_n for prime n - so this is the unique group. Recall that I claimed earlier that $\mathbb{Z}_3$ was the unique group with 3 elements - this is why.

Let's look back at the non-cycle 4th order group we discussed earlier with the Cayley table:

$$\begin{array}{c|cccc} * & e & a & b & c \\ \hline e & e & a & b & c \\ a & a & e & c & b \\ b & b & c & e & a \\ c & c & b & a & e \end{array} \tag{7.12}$$

This has subgroups $\{e, a\}$ and $\{e, b\}$ and $\{e, c\}$ which are all $\mathbb{Z}_2$ groups. Or, thinking more physically and recalling that this corresponds to the symmetries of a rectangle as sketched in Fig. 7.1, identity and any one of the transformations (e.g. rotation by π, reflection in the horizontal axis, reflection in the vertical axis) each forms a group because each of these transformations are self-inverse.

Exercise: What are the subgroups of C3v group? Does this make sense in terms of the symmetries of the Ammonia molecule, NH3?

A useful theorem in finite group theory is the reordering theorem:

Theorem 7.2.5 (Reordering theorem)**.** *Let G be a finite group and m one of its elements. The ensembles mG and Gm are a re-order of G.*

First lets check that this is true for an example we've just looked at - the rectangle symmetry group R_2. Suppose we take the set $G = \{e, a, b, c\}$ and multiply each element by the element $m = a$ to give $mG = \{a, a^2, ab, ac\}$. Then from the Cayley table of the group in Eq. 7.12 we get $mG = \{a, e, c, b\}$. This is just the original group reshuffled. As the group is Abelian the same applies for Gm.

This is the type of theorem where I almost feel that just staring and convincing yourself of it is the best way forward- as groups are closed multiplying through by a group element gives another group element and the requirement for each element have an inverse means that you always get a different element on multiplying through. Alternatively, one can more formally argue the following:

Demo. The map $x \to mx$ is surjective (i.e. all elements have an antecedent). Indeed for any $y \in G$, $m^{-1}y \in G$ (group property) and $m(m^{-1}y) = y$. The map $x \to mx$ is also injective (it maps distinct elements to distinct elements). For any $x \neq x'$, $mx \in G$ is different from mx'. Indeed, if $mx = mx'$ then $m^{-1}(mx) = m^{-1}mx'$ and $x = x'$. Hence the map is bijective and therefore a reordering. The proofs works in a similar way for the map $x \to xm$. (For more on the properties of functions see Appendix 7.14) □

Group Homomorphism and isomorphism The final important concept I will discuss in this section is that of group homomorphisms and isomorphisms. This formalises the important idea that I have been repeatedly hinting at but glossing over - the idea of superficially different looking groups being the same in some sense.

A group homomorphism, is a mapping between two groups which respects the group structure:

Definition 7.2.6 (Group homomorphism)**.** A function from a group $(G, *)$ to the group $(G', \star)$ is an application $f : G \to G'$ such that $\forall x, y \in G \quad f(x * y) = f(x) \star f(y)$.

It implies in particular that $f(e) = e'$, (where e and e' denote the respective neutrals of G and G') as well as $f(x^{-1}) = f(x)^{-1}$. For instance, it is always possible to create a morphism of any finite group to the trivial group by mapping all the elements to e'. A less trivial example is that the group Z_2 is homomorphic to $Z = \{\dots, -3, -2, -1, 0, 1, 2, \dots\}$ equipped with addition using $f(x) = 1$ for even numbers and $f(x) = -1$ for odd numbers for $x \in Z$.

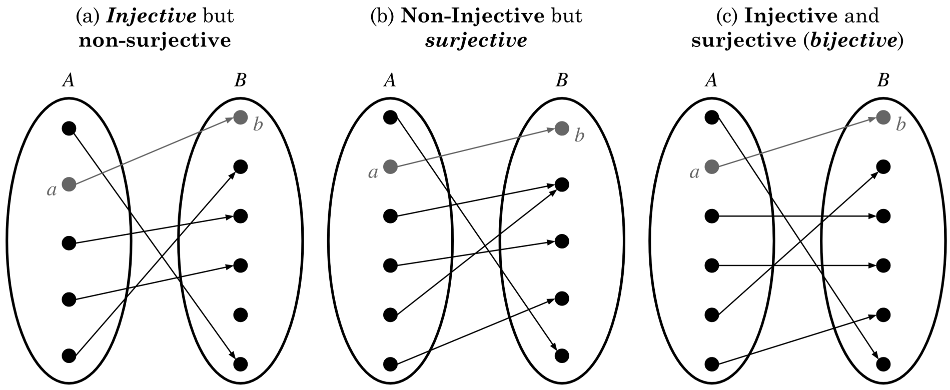


Figure 7.3: Diagram of injective, surjective and bijective functions: (Wiki page on functions).)

A homomorphism from $f : G \to G'$ can be bijective, i.e. be a map with a one-to-one correspondence between elements in the domain and range as sketched in Fig. 7.23. In this case, we call the mapping an isomorphism.

Definition 7.2.7 (Group isomorphism)**.** A group isomorphism is a function between two groups that sets up a one-to-one correspondence between the elements of the groups in a way that respects the given group operations.

If there exists an isomorphism between two groups, then the groups are called isomorphic. From the standpoint of group theory, isomorphic groups have the same properties and need not be distinguished. In the case of finite groups, this means that the groups have the same Cayley table. For example, $G = \{1, -1\}$ with $*$ standard scalar multiplication, $G = \{I, X\}$ or $G = \{I, \mathrm{SWAP}\}$ with $*$ matrix multiplication are isomorphic to $\mathbb{Z}_2$. Similarly, multiplication on the unit circle in the complex plane $[e^{i\phi}]$ and rotation around any single axis on the Bloch sphere, e.g. $[R_z(\phi)]$ where $R_z(\phi) = e^{-i\phi Z}$, are isomorphic to $U(1)$. (However, Z_2 is homomorphic, but not isomorphic, to Z equipped with addition).

Theorem 7.2.8 (Image of inverses and neutral element)**.** *If G is homomorphic to H by $f : H \to G$, then $e' = f(e)$ and $f(u^{-1}) = (f(u))^{-1}$*

Demo. Clearly, $f(e)f(u) = f(eu) = f(u)$ so the first property is proven. For the second, we write $f(u)f(u^{-1}) = f(uu^{-1}) = f(e) = e'$ so that the converse of $f(u)$ is $f(u)^{-1}$ □

7.3 Basic definitions and properties of representations

Let us now return to representations. As I mentioned earlier *groups* encode abstract symmetries but *representations* describe concrete realisations of those symmetries. Informally, a representation of a group captures the action of a group on a vector space (e.g. on quantum states). In particular, in a quantum context, it is a map from the elements of a group to a set of unitaries such that multiplication of that set of unitaries obeys the same properties as the original group. For example, the group Z_2 can be represented as $\{1, X\}$ and $\{1, \text{SWAP}\}$ acting on C^2 and $(C^2)^{\otimes 2}$ respectively. We can formally define the notion of a representation of a group via the notion of homomorphisms introduced above.

Definition 7.3.1 (Group representation)**.** A representation R of a group G on a vector space V is a group homomorphism from G to $GL(V)$, the general linear group [5] on V: i.e., $R : G \to GL(V)$. The dimension of a representation R is defined to be $\dim(R) = \dim(V)$.

We stress that formally a representation is by definition the *map* R. However, more informally the word representation is used in multiple ways. For example, informally you might hear someone discuss the $\{1, \text{SWAP}\}$ representation of $\mathbb{Z}_2$. Technically $\{1, \text{SWAP}\}$ is a group (that is isomorphic to $\mathbb{Z}_2$) and the representation is the map R such that $R(e) = I$ and $R(a) = \text{SWAP}$ (where the properties of a and e are captured by the $\mathbb{Z}_2$ Cayley table). As long as you remember that fundamentally it is the underlying map that is the representation, this casual way of speaking shouldn't cause too much confusion in practise[6].

Let us give a few examples:

Trivial representation. All groups admit a trivial representation (or the Identity representation): $\forall g \in G, R(g) = I$.

Examples representations for the parity group $Z_2 = \{e, a\}$.

- As we said before we have the representations $G = \{1, X\}$ and $G_{\text{SWAP}} = \{1, \text{SWAP}\}$ acting on C^2 and $(C^2)^{\otimes 2}$ respectively. You could also have[7] $G = \{1, Z\}$ on C^2.
- On $\mathbb{R}$ it has two representations: 1) the trivial representation $R(g) = 1$ for $g = e, a$, as well as 2) the representation $R(e) = 1, R(a) = -1$.
- The trivial representation $\{I\}$ can also of course be defined on a vector space of any dimension.

Examples representations for $O(3)$. Consider $O(3)$ the group of orthogonal matrices in dimension $d = 3$. We recall that this is the set of all 3×3 matrices M such that $MM^T = I$.

- The simplest representation, called the fundamental representation, is simply the set of all 3×3 orthogonal matrices.
- The morphism $R(g) = \det(M) = \pm 1$ is a representation of $O(3)$ on the vector space $\mathbb{R}$ (indeed $\det(AB) = \det(A)\det(B)$).

[5] The general linear group is the group of invertible linear transformations on a vector space V

[6] This subtlety is put nicely in Representation Theory for Geometric Quantum Machine Learning: *As an unfortunate feature of the subject, the word "representation" can equivalently refer to the group homomorphism R, the vector space upon which it acts V, or the image subgroup $R(G) \subset GL(V)$. Once one gets used to this, it is not as bad as it sounds: in practice, one often thinks of a representation as being the shared data of the vector space V and the linear action of G on that vector space.*

[7] This is in fact *equivalent* to the $G = \{1, X\}$ as they are related by a unitary transformation. More on equivalent transformations in a bit.

Fundamental representation of continuous groups. All continuous groups have the a 'fundamental' representation where the matrices in the group and the matrices in the representation coincide ("up to change of basis")[8].

Adjoint representation. Another important representation that is possible for any group is the adjoint representation. Thus far we have considered representations that map vectors to vectors, it is also possible to consider representations that map matrices to matrices. Let $V = M_2(\mathbb{C})$ denote the set of 2×2 complex matrices. The linear super-operator

$$A \mapsto U_g A U_g^\dagger \tag{7.13}$$

where $U_g = R(g)$ is a possible representation of G. For example, $U...U^\dagger$ for $U \in SU(2)$ is a representation of $SU(2)$.

So far we have spotted the representations corresponding to a symmetry group just by 'seeing them'. In fact, as I discussed earlier, the process often in physics goes the other way around. We know the symmetry at the level of the representation and then abstractify to identify the underlying group. But what about going the other way around - what if we have a group, and don't know any of its (non-trivial) representations, and want to find one?

Regular representation of finite groups. All finite groups admit what is known as the 'regular' representation as one of its representations.

Definition 7.3.2 (Regular representation)**.** For a finite group of order h, one can construct the so-called regular representation using $h \times h$ matrices as follows. First start from the following *reordered* Cayley table (here for $h = 3$):

$$C = \begin{array}{c|ccc} * & e & a^{-1} & b^{-1} \\ \hline e & e & a^{-1} & b^{-1} \\ a & a & e & ab^{-1} \\ b & b & ba^{-1} & e \end{array} \tag{7.14}$$

Now the representation can be done using the following matrices for $g \in G$: We use a matrix which is zero everywhere except for the position that corresponds to the group element in the Cayley table:

$$(R(g))_{ij} = \delta_{g,C_{ij}} \tag{7.15}$$

With this definition, e is represented by the identity matrix $R(e) = I$. It is easy to check that these matrices indeed follow the group algebra. You'll work through some examples of this in the problem sheet.

It is also possible to construct representations from a simpler (set of) already known representations.

[8]Note that although the matrices between the group G and its representatives $\{R_g : g \in G\} \subseteq \mathrm{GL}(V)$ are identical, we think of the abstract group and its representatives as conceptually distinct.

Equivalent representations. Consider a group G and a representation $R(g) \forall g \in G$. We define now $R'(g) = SR(g)S^{-1}$ where S can be any invertible matrix. This is a *similarity* transformation[9]. It is easy to see that similarity transformations of representations are still representations. It is straightforward to verify that $R'(g)$ is a representation of G (i.e., if $R(gh) = R(g)R(h)$ then $R'(gh) = SR(g)R(h)S^{-1} = SR(g)S^{-1}SR(h)S^{-1} = R'(g)R'(h)$).

Definition 7.3.3 (Equivalent representation)**.** Two representations D and D' are equivalent if they are related by a similarity transformation $R'(g) = SR(g)S^{-1}$.

Roughly speaking, representations are equivalent if we can transform one to the other by a linear invertible transformation. If what follows, we shall be mainly concerned by unitary representations and transformations. In this case $SS^\dagger = 1$ and $S^\dagger = S^{-1}$. This means that we shall consider two representations as equivalent if they simply correspond to a change of basis: $R'(g) = UR(g)U^\dagger$.

Tensor product representation. For example, consider two representations R_1 and R_2 for a group G, it is straightforward to verify (*check this!*) that the tensor product of their representations $R_1 \otimes R_2$, i.e. the set of matrices such that

$$R_1(g) \otimes R_2(g) \tag{7.16}$$

for each element g, is also a representation. For example, $\{I \otimes I, Z \otimes Z\}$ is a representation of Z_2 (in fact, $\{I^{\otimes k}, Z^{\otimes k}\}$ is a representation for any k).

Tensor product representations are fundamental in physics whenever we take the symmetry property of a single system and want to study the properties of a composite system. For example, suppose we have a system of n particles each of which are $SU(2)$ symmetric. In this case, we will be interested in the representation of $SU(2)$ on $(C^2)^{\otimes n}$, and so a natural choice is $SU(2)^{\otimes n}$.

Direct sum representation. Another useful composite representation, one that plays a key role in physics, is the direct sum representation.

Definition 7.3.4. Consider two representations R_1, R_2 of a group G acting on vector space V_1, V_2. The direct sum $R_1 \oplus R_2$ is a representation of G acting on $V_1 \oplus V_2$ defined by

$$(R_1 \oplus R_2)(g)(v_1, v_2) := (R_1(g)v_1, R_2(g)v_2), \quad \text{for all } g \in G. \tag{7.17}$$

Or, writing the matrices out explicitly, $R_1 \oplus R_2$ acting on $V_1 \oplus V_2$ we have:

$$(R_1 \oplus R_2)(g) := \begin{pmatrix} R_1(g) & 0 \\ 0 & R_2(g) \end{pmatrix}, \quad \text{for all } g \in G. \tag{7.18}$$

That this is indeed a representation follows straightforwardly from the block structure of Eq. (7.18). (If this isn't immediately clear to you, do work through it explicitly). We can also take the direct sum of the same representation, i.e., $R_1 \oplus R_1$, in which case we say that R_1 has multiplicity of two, and we write

$$(R_1 \oplus R_1)(g) = \begin{pmatrix} R_1(g) & 0 \\ 0 & R_1(g) \end{pmatrix} = I \otimes R_1(g), \quad \text{for all } g \in G. \tag{7.19}$$

[9]In linear algebra, two $n \times n$ matrices A and B are called similar if there exists an invertible n-by-n matrix P such that $B = P^{-1}AP$.

Notice that due to the block structure of a direct sum representation the action of an element of the representation structure of a group leave certain subspaces invariant. This will turn out to be very important.

Hopefully it is now clear how you can take simple representations of a group and create more complex ones. In many cases, we will in fact be more interested in going in the other direction. Taking a complex representation and trying to break it down into a simpler one. More concretely, one of the things representation theory is most useful for is *taking a representation (e.g. say a tensor one), and expressing it as a direct sum of representations on smaller subspaces*. We will discuss this in Section 7.6

7.4 A little bit on Lie Algebras

Lie groups (i.e. continuous groups) necessarily have uncountably many elements, in contrast to finite discrete groups, and this can make them a bit of a pain to work with. It is often convenient to work not at the level of the group elements / representations but instead at the level of the *generators* of the group elements. To motivate this switch let's start with an example.

7.4.1 Warm up example of $SO(3)$

Let us start by looking at the example of $SO(3)$ (i.e., rotations in 3D). Any rotation in 3D can be decomposed into rotations around the x, y and z axes respectively:

$$R_x(\theta) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & -\sin\theta \\ 0 & \sin\theta & \cos\theta \end{bmatrix}, R_y(\theta) = \begin{bmatrix} \cos\theta & 0 & \sin\theta \\ 0 & 1 & 0 \\ -\sin\theta & 0 & \cos\theta \end{bmatrix}, R_z(\theta) = \begin{bmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{bmatrix} \tag{7.20}$$

We want to find the set of matrices that *generate* these rotations. That is, the set of matrices J such that $e^{-i\theta J} = g$ for all $g \in G$. To do so it is helpful to look at small rotations and Taylor expand $e^{-i\theta J} = I - i\theta J + O(\theta^2)$. If θ is small, we see that the rotation around the z axis reads

$$R_z(\theta) \approx \begin{bmatrix} 1 & -\theta & 0 \\ \theta & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = I - i\theta \begin{bmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} = I - i\theta J_z \tag{7.21}$$

and so we can identify the generator

$$J_z := \begin{bmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}. \tag{7.22}$$

J_x and J_y can be found in the same manner. More generally, we see that if we perform an infinitesimal rotation around each axis with angles $\theta_x, \theta_y, \theta_z$, we have

$$\boldsymbol{V'} \approx (I - i\theta_x J_x)\,(I - i\theta_y J_y)\,(I - i\theta_z J_z)\,\boldsymbol{V} \approx (I - i\boldsymbol{\theta}\cdot\boldsymbol{J})\,\boldsymbol{V} \tag{7.23}$$

with

$$\boldsymbol{\theta} = \begin{bmatrix} \theta_x \\ \theta_y \\ \theta_z \end{bmatrix} \tag{7.24}$$

$$J_x = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{bmatrix}, J_y = \begin{bmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{bmatrix}, J_z = \begin{bmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \tag{7.25}$$

Since we can always decompose large rotation as a successions of small ones, this means that we should be able to integrate over these infinitesimal moves [10], so that for any $R(\boldsymbol{\theta}) \in SO(3)$ we have

$$R(\boldsymbol{\theta}) = e^{-i\boldsymbol{\theta}\cdot\boldsymbol{J}} \tag{7.26}$$

In fact, this can be checked directly by expanding the exponential. The matrices $\{iJ_x, iJ_y, iJ_z\}$ are called the "(infinitesimal) generators" of the SO(3) group.

[10] Note that $e^x = \lim_{n\to\infty}(1 + \frac{x}{n})^n$.

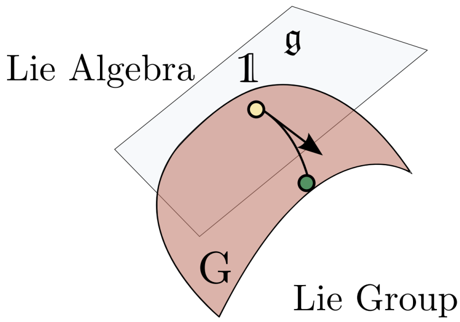


Figure 7.4: Geometric visualisation of definition of Lie Algebra (from Representation Theory for Geometric Quantum Machine Learning). Continuous groups are manifolds and manifolds are complicated non-linear objects to analyse. But we can construct smooth paths in the group, similarly to how one can construct paths along surfaces. That is, we can take derivatives along paths in the group similarly to taking derivatives of paths on surfaces. The structure that stores the information of "directional derivatives of continuous group paths" is the *Lie algebra* $\mathfrak{g}$. More concretely, the Lie algebra $\mathfrak{g}$ is defined as the tangent plane at identity of the manifold (Lie group) G. So, paths in G can be differentiated at I to give directional derivatives in $\mathfrak{g}$, and paths in $\mathfrak{g}$ can be exponentiated to give paths in G, just as in solutions to linear ordinary differential equations. For instance, if for an element of the algebra $X \in \mathfrak{g}$ we define a path $g = e^{\theta X} \in G$, then $\frac{d}{d\theta} g(\theta)\big|_{\theta=0} = Xe^{\theta X}|_{\theta=0} = X$. For this geometric picture it's simpler not to explicitly factor out the $-i$ term but the story is the same either way.

This is actually a generic phenomenon for Lie groups. Since they are differentiable, it is always possible to write an element g of a Lie group G as the exponential of an element J of the corresponding Lie Algebra $\mathfrak{g}$. That is,

$$\mathfrak{g} = \{J | e^J \in G\} . \tag{7.27}$$

This switch can also be understood geometrically as sketched in Fig. 7.4.

Spinning things around, we can recover any $J \in \mathfrak{g}$ by starting with a one-parameter subgroup $e^{-i\theta J} \subseteq G$ and taking derivatives at the identity $I = e^0$:

$$-J = \frac{d}{dt}(e^{-\theta J})\bigg|_{\theta=0} . \tag{7.28}$$

Alternatively, using the Taylor expansion $g = I - \theta J + O(\theta^2)$ where $J \in \mathfrak{g}$, the matrix equations defining the Lie group G induce equations defining the Lie algebra $\mathfrak{g}$. If G is a unitary group (as is typical in quantum settings), then we have $g^\dagger g = I$ and so

$$(I - \theta J + O(\theta^2))^\dagger (I - \theta J + O(\theta^2)) = I. \tag{7.29}$$

Equating θ terms, we see that $J^\dagger = -J$, meaning the Lie algebra $\mathfrak{u}(d)$ of a unitary group $U(d)$ consists of skew-Hermitian matrices J with the standard matrix commutator[11].

Similarly, to how Lie groups are a (continuous) set equipped with a group operation for combining elements, a Lie algebra is a vector space equipped with an operation for combining

[11] The Lie Algebra can also be defined as $\mathfrak{g} = \{J | e^{iJ} \in G\}$. This is, for example, the definition Florent Krzakala and Howard Georgi use. In this case the generators of the Lie Algebra consists of Hermitian matrices. In an earlier version of these notes I jumped between the two definitions slightly. I'm now going to try and be consist with the version in Eq. (7.27) but its good to be aware that both versions are possible and only really differ in terms of where the i's appear.

elements. Whereas the relevant group operation (in a quantum context) is typically matrix multiplication, the relevant operation for an algebra (in a quantum context) is commutation [12].

To see this consider two group elements $g_1 = e^{-i\theta_1 J_1}$ and $g_2 = e^{-i\theta_2 J_2}$. As the group is closed we have $g_1 g_2 = g'$ where g' is some other element in the group. Thus we have:

$$g_1 g_2 = e^{-i\theta_1 J_1} e^{-i\theta_2 J_2} = g' = e^{-i\boldsymbol{\theta}'.\boldsymbol{J}} \tag{7.30}$$

for some $\boldsymbol{\theta}'$. Now the left hand side of the above equation can be evaluated via the Baker-Campbell-Hausdorff (BCH) formula:

$$e^{-i\theta_1 J_1} e^{-i\theta_2 J_2} = e^{-i\theta_1 J_1 - i\theta_2 J_2 - \frac{\theta_1\theta_2}{2}[J_1,J_2] + i\frac{\theta_1^2\theta_2}{12}[J_1,[J_1,J_2]] + i\frac{\theta_2^2\theta_1}{12}[J_2,[J_2,J_1]]) + \dots} . \tag{7.31}$$

Thus we see that the generator J', of this new group element g', is composed of a linear combination of the original J_1 and J_2 and a bunch of their nested commutators. In particular, to first order in θ_1 and θ_2 we have

$$i\boldsymbol{\theta}'.\boldsymbol{J} = i\theta_1 J_1 + i\theta_2 J_2 + \frac{\theta_1\theta_2}{2}[iJ_1, iJ_2], \tag{7.32}$$

and so $i\boldsymbol{J} = (iJ_1, iJ_2, [iJ_1, iJ_2])$. Let us look at the commutation relation of these generators for $SO(3)$. We find:

$$[J_i, J_j] = i\varepsilon_{ijk} J_k \tag{7.33}$$

with ε_{ijk} the Levi-Cevita symbol. Thus we see that $[iJ_1, iJ_2] = -iJ_3$ and so $\boldsymbol{J} = (J_1, J_2, J_3)$ as expected. Note that in this case, higher order nested commutators of J_1 and J_2 just give, up to constant multiplicative factors, J_1, J_2 or J_3. Thus we see, as we saw before, that iJ_1, iJ_2 and iJ_3 form a basis for the so(3) Lie algebra [13] and so(3) is said to be a 3-dimensional Lie algebra.

7.4.2 Definitions and basic properties

Ok we've run through an example that has hopefully highlighted different aspects to a Lie algebra now let's take a step back and recap. We first pointed out that exponentiation of every element J of the Lie algebra leads to an element of the Lie group with

$$\mathfrak{g} = \{J | e^J \in G\}. \tag{7.34}$$

We then saw that (given the BCH formula) any element in the Lie algebra can be generated from a linear combination of nested commutators of other elements of the algebra [14]. That is, the elements of a Lie algebra form a vector space. It is worth stressing that the fact a Lie algebra is a *vector space* is part of their appeal. As lie algebras are vector spaces we can tackle them via linear algebra (which is generally less painful than differential geometry). This means when faced with a problem with a Lie group symmetry it is often worth passing to the Lie algebra to try and analyse it and then translate the conclusions back to the level of the Lie group.

While it is possible to define a Lie algebra via its Lie group, in quantum contexts it is common to start with generators and use them to define the algebra directly through the nested

[12] However, where as multiplication generates another group element; here the commutator generates another basis operation of the algebra and to generate the full set one needs to consider linear combinations of the basis elements.

[13] Note we use lower case letters or if we're feeling fancy the 'mathfrak' font to denote the Lie algebra corresponding to a Lie group G. So, so(3) or equivalently $\mathfrak{so}(3)$ denotes the Lie algebra corresponding to SO(3).

[14] Turning this around a set S of operators such that a Lie algebra $\mathfrak{g}$ is spanned (as a vector space) by all nested commutators of elements of S form a set of *generators* for an algebra.

commutator relation similar to the so(3) example above. This way of defining a Lie algebra is often known as the 'dynamical Lie Algebra' because it emphasises the role of the generators as the generator of dynamics. Pennylane have a nice tutorial on this.

Definition 7.4.1 (Dynamical Lie Algebra)**.** Given a system with a set of Hermitian operators $\mathcal{G} = \{iJ_k\}_{k=0}^{K}$, the *Dynamical Lie Algebra (DLA)* $\mathfrak{g}$ is the sub-algebra of $\mathfrak{su}(d)$ spanned by the repeated nested commutators of the elements in $\mathcal{G}$, i.e.,

$$\mathfrak{g} = \mathrm{span}\{iJ_0, \dots, iJ_K\}_{\mathrm{Lie}} \subseteq \mathfrak{su}(d), \tag{7.35}$$

where $\{\}_{\mathrm{Lie}}$ denotes the Lie closure, i.e., the set obtained by repeatedly taking the nested commutators between the elements in $\mathcal{G}$.

The above definition of a Lie algebra will suffice for our purposes. But just for completeness, let us note that more generally they can be defined as follows:

Definition 7.4.2. A *Lie algebra* is a vector space $\mathfrak{g}$ over a field $\mathbb{F} \in \{\mathbb{C}, \mathbb{R}\}$ (for us usually over $\mathbb{C}$) with a *Lie bracket* $[\cdot,\cdot] : \mathfrak{g} \times \mathfrak{g} \to \mathfrak{g}$, which satisfies the following axioms holding for all $X_1, X_2, X_3 \in \mathfrak{g}$ and $a, b \in \mathbb{F}$,

1. *Antisymmetry*: $[X_1, X_2] = -[X_2, X_1]$.
2. *Bilinearity*: $[aX_1 + bX_2, X_3] = a[X_1, X_3] + b[X_2, X_3]$.
3. *Jacobi Identity*: $[[X_1, X_2], X_3] + [[X_2, X_3], X_1] + [[X_3, X_1], X_2] = 0$.

The standard commutator $[A, B] = AB - BA$ satisfies this properties and is generally the only Lie bracket that will matter in most quantum settings.

How does this link back to the previous definition? Finally, well if we are just interested in the standard commutator then a convenient way of identifying a Lie algebra in practise is via identifying a set of generators and their commutation relations. The vector space corresponding to the algebra is then defined via Eq. (7.35). For instance, the Lie algebra $\mathfrak{so}(3)$ of the Lie group $SO(3)$ can be expressed by writing angular momentum operators L_x, L_y, L_z and their commutation relations $[L_i, L_m] = i\hbar \sum_n \epsilon_{imn} L_n$. More generally, given any three elements of a Lie algebra J_a, J_b, J_c the constants f_{abc} such that

$$[J_a, J_b] = i f_{abc} J_c \tag{7.36}$$

are known as the structure constants and completely determine the algebra.

7.4.3 Representations of Lie groups and algebras

We need to be a little careful with how we speak here. Similarly to how groups encode an abstract symmetry and representations their physical realisation, Lie algebras encode abstract symmetries and their representations their physical realisations. And technically, representations of Lie Algebra's are the map r from the elements of the Lie Algebra to matrices used to represent it which satisfy the same Lie Algebra. Again, in casual speaking we often just refer to the matrices themselves as the representation. More formally:

Definition 7.4.3. Let $\mathfrak{g}$ be a Lie algebra and V be a finite dimensional vector space. A representation r of $\mathfrak{g}$ acting on V is a map $r : \mathfrak{g} \to \mathfrak{gl}(V)$ that is a Lie algebra homomorphism, a linear map satisfying

$$r([X, Y]) = [r(X), r(Y)], \text{ for all } X, Y \in \mathfrak{g}. \tag{7.37}$$

The *dimension* of the representation r is defined by $\dim(r) = \dim(V)$.

$$\begin{tikzcd}
\boxed{\text{Group, SO(3)}} \arrow[r, dash] \arrow[d, dash] & \boxed{\text{Representation of SO(3)}} \arrow[d, dash, dashed, "?"'] \\
\boxed{\text{Lie Algebra, } \mathfrak{so}(3)} \arrow[r, dash] & \boxed{\text{Representation of } \mathfrak{so}(3)}
\end{tikzcd}$$

While representations of groups are unitaries, representations of Lie algebras broadly correspond to the Hamiltonians (i.e., Hermitian operators) that generate those unitaries. In terms of the SO(3) example, the matrices J_x, J_y, J_z are a basis for the representation of the Lie Algebra of $\mathfrak{so}(3)$: they define a particular representation, in dimension 3, of matrices that satisfies the commutation relation of $\mathfrak{so}(3)$. However, other representations of $\mathfrak{so}(3)$ are possible (after all, this is a VERY common commutation relation: all spin moments operators will satisfy it!).

An important question now arises: we see that we have one representation of the Lie Algebra (the J) and if we exponentiate it, we find one representation of the Group (the R). However, we know that there are many representation of $SO(3)$ (in many dimensions).

So is it true that ANY representation [15] of the Lie Algebra will lead, upon exponentiation, to a representation of the group?

The answer to this question is, unfortunately, **NO, in general!**, but **YES if the group is simply connected**. Topology plays an important role here: it is only for *simply connected* groups that any representation of the Lie Algebra is also a group representation.

A manifold is called *simply connected* if every loop can be contracted without leaving the surface. Intuitively, this corresponds to a space that has no disjoint parts and no holes that go completely through it, because two paths going around different sides of such a hole cannot be continuously transformed into each other. For example, the surface of a sphere is simply connected but the surface of a donut is not as shown in Fig. 7.5.

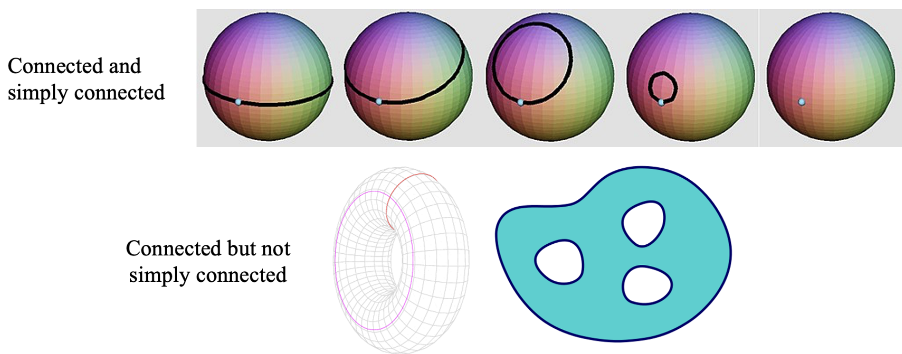


Figure 7.5: Some pictures from the wiki page on simply connected spaces.

Why is it so important that the topology of the group is simply connected? This has to do with analytic continuation and the fact that one can go from a succession of infinitesimal moves to a large one in a single, well-defined, way. This is only possible for simply connected topologies. The result is that if G is simply connected, there is a one-to-one correspondence

[15]Note, I am speaking casually here and referring to exponentiating the matrices themselves here i.e. exponentiating $r(X)$, and not exponentiating the map r (whatever that would mean).

between their representations. But if we relax the simply connected assumption, the power of this theorem weakens but not too much - locally there is still a correspondence between their representations. Spelling this out explicitly is beyond the remit of this course but, if you are interested, I provide more formal statements on this link in Appendix 7.19

7.4.4 The Bloch Sphere revisited: SU(2) versus SO(3)

Let us start by showing that any representation of SO(3) is a representation of SU(2).

To do so we consider a representation of SU(2) in $\boldsymbol{v} \in \mathbb{R}^3$. For any point in $\boldsymbol{v} \in \mathbb{R}^3$, we associate the following $d = 2$ Hermitian and zero trace matrix.

$$M(\boldsymbol{v}) = \begin{bmatrix} z & x+iy \\ x-iy & -z \end{bmatrix} = x\sigma_x + y\sigma_y + z\sigma_z = \boldsymbol{v}.\boldsymbol{\sigma} \tag{7.38}$$

where $\boldsymbol{v} = (x, y, z)$. Now, let us look how SU(2) transforms these matrices. We define the transformation as

$$M' = f_U(M) = UMU^{-1}\,. \tag{7.39}$$

Clearly, such transformation respects the SU(2) structure. Indeed,

$$f_U(f_V(M)) = U(VMV^{-1})U^{-1} = UVM(UV)^{-1} = f_{UV}(M) \tag{7.40}$$

Additionally, these transformations keep the trace zero and preserve the hermitian property ($(U\sigma U^\dagger)^\dagger = U\sigma U^\dagger$ and $\mathrm{Tr}[U\sigma U^\dagger] = \mathrm{Tr}[U^\dagger U\sigma] = \mathrm{Tr}[\sigma] = 0$ for any Pauli σ), and so the transformation M' can also be expressed as the linear combination of σ_x, σ_y and σ_z:

$$M' = \begin{bmatrix} z' & x'+iy' \\ x'-iy' & -z' \end{bmatrix} = x'\sigma_x + y'\sigma_y + z'\sigma_z = \boldsymbol{v}'.\boldsymbol{\sigma}\,. \tag{7.41}$$

This means that our transformation on M implies, implicitly, a transformation in $3d$ with $\boldsymbol{v}' = f_U^{3d}(\boldsymbol{v})$. This transformation is continuous and linear ($M_1' + M_2' = U(M_1 + M_2)U^{-1}$. Additionally, it also preserves the determinant of M (as $\det(M') = \det(UMU^\dagger) = \det(U)\det(M)\det(U^\dagger) = \det(M)$, and thus it preserves the length of the 3d vector $\boldsymbol{v}$. In this case it can only be rotation and/or mirrors. But mirrors are NOT continuous, and thus this means that $f_U^{3d}(\boldsymbol{v})$ is a rotation of the point $\boldsymbol{v}$.

We have thus created an interesting bridge: $f_U^{3d}(\boldsymbol{v})$ is just implementing rotations so that

$$f_U^{3d}(\boldsymbol{v}) = R(U)\boldsymbol{v} \tag{7.42}$$

Therefore, we have made (implicitly) a map between the SU(2) group to the SO(3) group: the matrices R(U) (which are just the rotation matrices of SO(3)) are a representation of SU(2), since they follow the $f_U^{3d}(\boldsymbol{v})$ transformation, and thus the SU(2) composition rule. **In other words a representation of SO(3) is a representation of SU(2).** This is essentially just a rephrasing of the derivation of the Bloch sphere in the very first lecture.

However, the opposite is not true! In fact, it is easy to see that this relation is not an isomorphism (Definition 7.2.7), because U and $-U$ have the exact same effect [16] in eq.(7.39) and so there is not a one-to-one correspondence between the elements of the group. Therefore, both of U and $-U$ have the same representation in SO(3): there are multiple elements of SU(2) for

[16] Technically this example only works for even dimensional problems. As U is in SU(n) then $\det(U) = 1$ and so $\det(-U) = \det(-I)\det(U) = 1$ if n is even. I only mention in case you were confused by this.

one element of SO(3). Therefore: **a representation of SU(2) is not a representation of SO(3).**[17]

Notice, however, that these elements differ only by a minus sign. We say that SU(2) is the *double cover* of SO(3) in that every element of SO(3) has two corresponding elements of SU(2) (i.e. ones corresponding to $+U$ and $-U$). Alternatively, a representation of SU(2) is what is known as a *projective representation* of SO(3): namely a set of operators that satisfy the homomorphism property up to a constant.

Definition 7.4.4 (Projective group representation)**.** A projective representation of a group G on a vector space V is a group homomorphism $R : G \to GL(V)$ up to a constant. That is, a morphism from a group $(G, *)$ to the group $(G', \star)$ is an application $f : G \to G'$ such that $\forall x, y \in G \quad f(x * y) = \lambda_{xy} f(x) \star f(y)$ for some constant λ_{xy}.

The fact that some mathematical objects transforms with SU(2) rather than SO(3) is a deep consequence of the laws of quantum mechanics. It tells us that it is possible that some object will transform with $SU(2)$ upon rotation! We know these objects: half integer spins!

Ok but what is going on at the level of the Lie Algebras? Well to move from a representation of a Lie group G to a representation of the Lie algebra $\mathfrak{g}$, we take derivatives of paths and evaluate at the identity. We have just seen that $SU(2)$ is homeomorphic to the 3-sphere, it is a 3 dimensional real manifold, and so its Lie algebra $\mathfrak{su}(2)$ is a 3 dimensional real vector space. It thus suffices to find 3 linearly independent tangent vectors, which we can do by taking derivatives of parameterized paths and evaluating at the identity I. Since we have explicit rotation paths which are I when $\theta = 0$, let us use those:

$$\begin{aligned}
\frac{d}{d\theta} R_x(\theta)\bigg|_{\theta=0} &= \frac{d}{d\theta} e^{-i\sigma_x\theta/2}\bigg|_{\theta=0} = -i\frac{1}{2}\sigma_x \\
\frac{d}{d\theta} R_y(\theta)\bigg|_{\theta=0} &= \frac{d}{d\theta} e^{-i\sigma_y\theta/2}\bigg|_{\theta=0} = -i\frac{1}{2}\sigma_y \\
\frac{d}{d\theta} R_z(\theta)\bigg|_{\theta=0} &= \frac{d}{d\theta} e^{-i\sigma_z\theta/2}\bigg|_{\theta=0} = -i\frac{1}{2}\sigma_z
\end{aligned}$$

Thus a possible representation for the Lie Algebra for su(2) is:

$$\left\{\frac{i}{2}\sigma_x, \frac{i}{2}\sigma_y\,, \frac{i}{2}\sigma_z\right\} \tag{7.43}$$

which obey the commutation relations

$$\left[\frac{1}{2}\sigma_i, \frac{1}{2}\sigma_j\right] = i\varepsilon_{ijk}\frac{1}{2}\sigma_k\,. \tag{7.44}$$

the same commutation relations as the J_x, J_y and J_z operators in the so(3) algebra. Therefore, we see that the su(2) Lie algebra is isomorphic to the so(3) Lie algebra! These groups have a deep relationship! Note the factor of 1/2 in the exponent, which was slightly mysterious in the first lecture, ensures this isomorphism between the two algebras. This factor also ensures that SU(2) is the double cover of SO(3). If we recall that

$$U(\theta) = e^{\frac{i\boldsymbol{v}.\boldsymbol{\sigma}}{2}} = \cos(\theta/2)I + i\sin(\theta/2)\boldsymbol{v}.\boldsymbol{\sigma} \tag{7.45}$$

[17] The more trivial example of this is that we have any group G is homomorphic to the trivial group. But, the trivial group is not homomorphic to G.

we see that for $\theta = 2\pi$ we have $U(2\pi) = -I$ and we need $\theta = 4\pi$ to regain $U(4\pi) = I$. That is, $U(\theta)$ and $U(\theta + 2\pi)$ are two different unitaries that correspond to the same Bloch vector.

If you were wondering how this all links back to groups being connected versus simply connected. Well SU(2) is simply connected and SO(3) is connected by not simply connected [18]. This means that the groups can share the same representation at the level of the lie algebra but only in the case of su(2) does this strictly lift to a representation of the group SU(2).

That all gets a little subtle but the punchline is: SU(2) and SO(3) have isomorphic Lie Algebras (su(2) and so(3)). Any representation of SO(3) is a representation of SU(2) but not vica versa.

[18] This is because there is an orientation component associated with SO(3) that you do not have with SU(2) and so, in handwavey terms, a rotation by 2π leads to a twist and so is not contractable. However, as $2 \times 2\pi$ rotation undoes this twist and so is contractable. I appreciate this is subtle and my answer has been very quick here - if you want to understand this better geometrically/pictorially I recommend this youtube video and this intuitive paper. For a deeper dive into this topic, and other topics on Lie Groups and Lie Algebras, I've been recommended this youtube series.

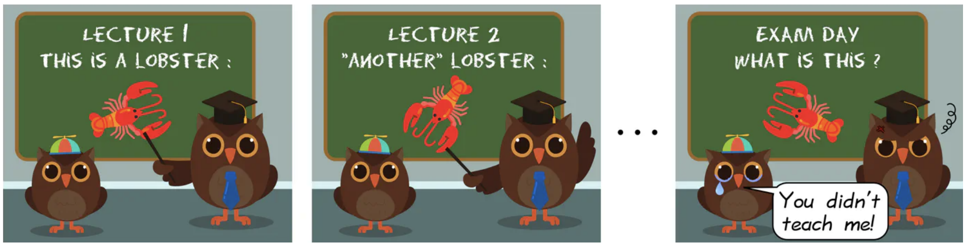


Figure 7.6: Why symmetry considerations are important for any learning task (image taken from this blog post).

7.5 (Quantum) Machine Learning Example

Ok time for a brief interlude from all the maths. Statistically, many of you taking this course will end up working on a mix of machine learning, data science and artificial intelligence at some point in your careers (whether you stay in physics or venture into the real world). As such I want to highlight to that symmetry considerations and therefore group theory can be really important in these areas. One thing that is also nice about these examples, unlike some more physics heavy examples which we will discuss later, is that we already have enough of the theoretical tools laid out to look at this application now.

So, why is symmetry important in machine learning? This is explained very nicely in this blog post which I'll draw from here. In particular, let's start with everyone's favourite example of a machine learning task: classifying images to decide if they include cats of dogs (Fig. 7.7). (If you want a less inane task consider trying to classify whether an images of tumours contain cancerous cells. Or whether images of galaxies contain supernova.)

Figure 7.7: Task: train a classifier to decide if an image contains a cat or a dog. The classifier is trained on a data set $\{(x_i, y_i)\}_{i=1}^{N}$ composed of a set of N images (x_i) and a corresponding label (y_i).

There are many different transformations one can perform to an image of a cat that still leave it as a picture of a cat - e.g. you can rotate it or reflect it and you are still left with an image of a cat (Fig. 7.8).

We want our classifier to be *invariant* under these symmetry transformations. In the context of image processing (or modelling molecules or materials) these symmetry transformations will typically be geometric transformations. Beyond image classification other symmetry transformations, such as permutation invariance, can become important. And, of course, mathematically all these symmetry transformations can represented by the actions of elements of a symmetry group.

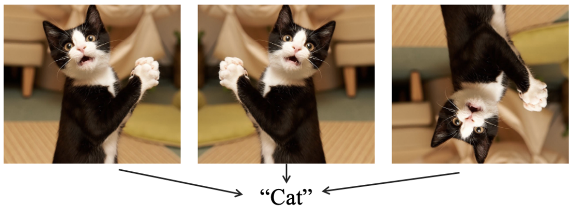


Figure 7.8: A picture of a rotated cat or flipped cat is still a picture of a cat.

7.5.1 Invariance versus equivariance.

An important distinction in the context of symmetry in machine learning is that between *invariance* and *equivariance*.

A function is *invariant* to a transformation if the function is left unchanged when its input is being acted on by the transformation group. This was the case for function (i.e. the model) classifying whether an image contains a cat. It would also be the case for a function predicting the ground state energy of a molecule as shown in Fig. 7.9.

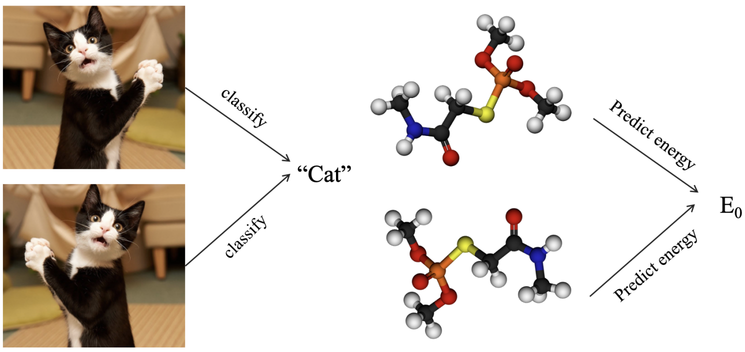


Figure 7.9: Examples of invariant functions.

Let's try to make this a bit more formal. We consider a function $f : X \to Y$ (e.g. the classification or energy prediction functions in the examples above) and a *symmetry group* G (e.g. rotations). Let $R_X(g)$ be a representation of G on X. The function f is then said to be G-*invariant* if

$$f(R_X(g) \cdot x) = f(x) \quad \forall g \in G, x \in X, .$$

On the other hand, a function is *equivariant* if the function's output transforms in the same way as its input. When this is the case it does not matter whether you first apply the transformation to the input and then function, or vice versa. That is, the function and the transformation commute as shown in Fig. 7.10.

Mathematically, a function is *equivariant* if

$$f(R_X(g)x) = R_Y(g)f(x) \quad \forall g \in G, x \in X\,, \tag{7.46}$$

where we note that X and Y are in general different spaces so the representations of the group actions on those two spaces, denoted R_X and R_Y respectively, may differ.

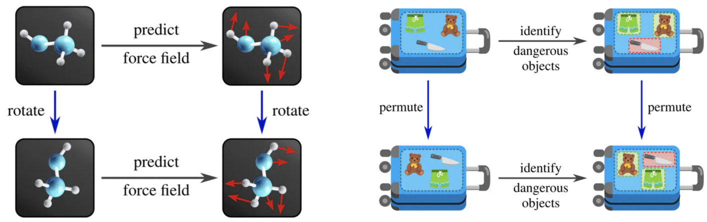


Figure 7.10: Examples of equivariant functions. (Image taken from this blog post)

7.5.2 Invariance and equivariance in quantum machine learning

I was torn whether to run through the maths here in a classical or quantum context. In the end I have settled on working through an example from quantum machine learning because i. this is a quantum course and so ii. based on what we have covered so far this semester I think the quantum case is simpler to understand. However, I should stress that no one knows yet if/where quantum machine learning will be useful. Therefore you should see this primarily as a pedagogical example. Here are some references if you are interested in seeing this discussion phrased in the example of classical neural networks: a blog post and textbook, an introductory article, and a tutorial with code snippets. I'm going to largely work from here: Representation Theory for Geometric Quantum Machine Learning.

Before working through this, you might find it helpful to first look back over to the section on quantum machine learning in Chapter 6. There we considered the binary classification problem sketched in Fig. 7.11.

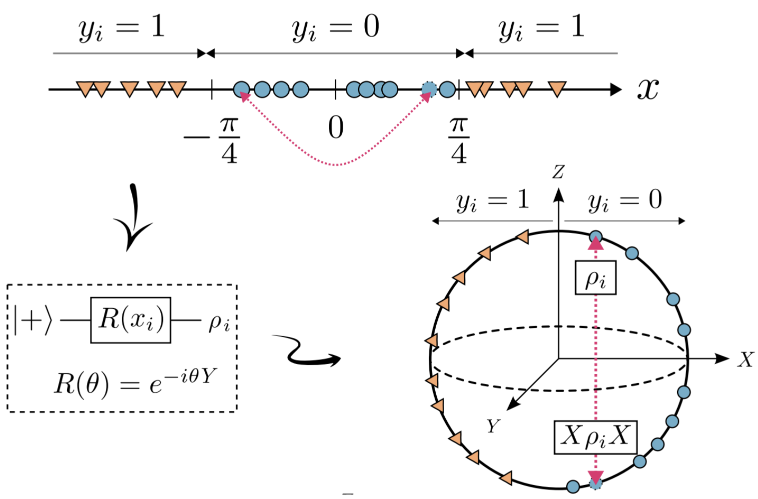


Figure 7.11: Binary classification problem using a single qubit encoding. The pink line denotes the symmetry transformation that leaves the data label invariant. (Image from here).

More generally, we can imagine a quantum machine learning classification model as being composed of two steps:

1. **An optional embedding.** Data x is embedded into a quantum state via a parameterized map e.g. $\rho_x = U(x)\rho_0 U(x)^\dagger$ where ρ_0 is some initial state and $U(x)$ is a parameterized unitary (i.e. circuit).

This embedding is optional as one can also consider quantum classification problems where the data is given to you already in the form of quantum states. For example, classifying pure versus mixed quantum states.

2. **Define and train a quantum model.** A general quantum model takes k copies of an input state ρ_x, processes it via a parameterized quantum circuit (PQC)[19] $U(\theta)$ and then performs a measurement M_x (which could depend on the input x):

$$h_\theta(\rho_x) := \mathrm{Tr}[U(\theta)\rho_x^{\otimes k}U(\theta)^\dagger M_x]\,. \tag{7.47}$$

This output is typically a real number, it can be turned into a label for classification e.g. via the sign function, e.g. $y = sign(h_\theta)$.

In this context, a quantum model is called invariant if the action of a unitary group G is said to leave the data labels y_x invariant, i.e. if

$$h_\theta(V\rho_x V^\dagger) = h_\theta(\rho_x)$$

for all ρ_x with labels y_x, for all θ, and for all unitaries $V \in G$. Let us stop and make a few comments. Firstly, label invariance trivially holds if the states are invariant under the symmetry i.e., if $V\rho_x V^\dagger = \rho_x$. However, this need not be the case! It is possible for the states $V\rho_x V^\dagger$ and ρ_x to be different but the label the same. Thus this is a wider class of symmetries than state symmetries.

So how could you go about constructing an *invariant* quantum model?

The first thing to do [20] is make your parameterized quantum circuit *equivariant*. Let

$$\mathcal{W}_\theta(\rho^{\otimes k}) := U(\theta)\rho^{\otimes k}U^\dagger(\theta) \tag{7.48}$$

denote the function corresponding to the parameterized quantum circuit applied to k copies of the input data state. Then, to ensure that $\mathcal{W}_\theta$ is equivariant, we require that

$$\mathcal{W}_\theta(V^{\otimes k}\rho^{\otimes k}(V^\dagger)^{\otimes k}) = V^{\otimes k}U(\theta)\rho^{\otimes k}U^\dagger(\theta)(V^\dagger)^{\otimes k} \quad \forall\ V \in G, \quad \forall\ \theta\,, \tag{7.49}$$

(We have simply plugged $\mathcal{W}$ and the adjoint representation $R_X(g)(...) = R_Y(g)(...) = V^{\otimes k}...(V^\dagger)^{\otimes k}$ into Eq. (7.46)). This condition is equivalent to requiring that the PQC commutes with all group elements

$$[V^{\otimes k}, U(\theta)] = 0 \quad \forall\ V \in G, \quad \forall\ \theta\,. \tag{7.50}$$

The second step is to pick your measurement so that it commutes with the group action

$$[V^{\otimes k}, M] = 0 \quad \forall\ V \in G\,. \tag{7.51}$$

While not formulated in precisely the form of Eq. (7.46) this commutation constraint can be also viewed as form of equivariance condition on the measurement operator.

[19] Also known as a *quantum neural network* (QNN).
[20] Note, this isn't the only way you could go about making your model invariant but it is the only way we will discuss here.

It is straightforward to check that these conditions really do lead to invariant quantum models:

$$\begin{aligned} h_\theta(V\rho_i V^\dagger) &= \mathrm{Tr}[\mathcal{W}_\theta((V\rho_i V^\dagger)^{\otimes k})M_i] \\ &= \mathrm{Tr}[(V^{\otimes k'}\mathcal{W}_\theta(\rho_i^{\otimes k})(V^\dagger)^{\otimes k'})M_i] \\ &= \mathrm{Tr}[\mathcal{W}_\theta(\rho_i^{\otimes k})(V^\dagger)^{\otimes k'}M_i V^{\otimes k'}] \\ &= \mathrm{Tr}[\mathcal{W}_\theta(\rho_i^{\otimes k})M_i] \\ &= h_\theta(\rho_i), \quad \forall\ V \in G. \end{aligned} \tag{7.52}$$

The model is invariant as claimed!

Quoting from here: *Conceptually, we can think of equivariant quantum neural networks as passing the action of the symmetry from their input, to their output, while equivariant measurements lead to models that absorb the action of the symmetry.*

For example, in our binary classification task considered in Fig. 7.11 the labels are invariant under bit flip, i.e. under $\{I, X\}$ (as sketched by the pink line). Thus to construct an invariant model we should use a parameterized quantum circuit and measurement operator that commutes with X and I. Thus we see immediately that our measurement operator M should be of the form $M = X$. Similarly, the equivariant parameterized quantum circuit consists only of rotations around X. As these trivially leave the measurement operator $M = X$ invariant we now see that for this simple example there is no need even to train.

Let us now consider a slightly less trivial example. Consider the binary classification task shown in Fig. 7.12 where the inputs are now two coordinate vectors, $x_i = (x_i^1, x_i^2)$ and the output label y_i depends only of the values x_i^1, x_i^2 and not their ordering (e.g., (x_i^1, x_i^2) and (x_i^2, x_i^1) have the same label). That is, the output label is invariance under permutations of the inputs, i.e. under the group $\{I, \mathrm{SWAP}\}$.

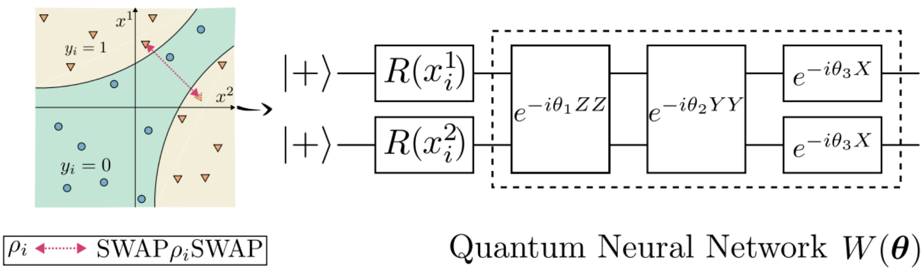


Figure 7.12: Binary classification problem for data living in a two-dimensional plane. (Image from here).

We can solve this classification using a two qubit model. The qubits are both initialized in the $|+\rangle$ state as previously and each input is encoded by applying a rotation of x_i^j about the Y axis on qubit j for $j = 1, 2$ (as shown in Fig. 7.12). For an invariant model we need to use an equivariant parameterized quantum circuit and measurement. This constraint on the measurement operator is relatively simple - we just need a measurement operator that commutes with the SWAP operator - a natural choice would be an operator of the form $M = \alpha_x X \otimes X + \alpha_y Y \otimes Y + \alpha_z Z \otimes Z$ where the α parameters could either be fixed or trainable. Similarly, the parameterized quantum circuit needs to commute with the SWAP operator for all θ. How do we ensure this in practise?

In general finding all the unitaries $U(\theta)$ that commute with all the representations V of the elements of the symmetry group G might seem rather challenging. But this is where the relationship between Lie algebras and Lie groups comes in handy. I'll quote from here:

We can use the trick of passing to the Lie algebra, solving there, and going back to the group. Explicitly, let us consider the case where $U(\theta)$ is composed of a single "layer", which is a fancy way of saying that $U(\theta) = e^{-i\theta H}$, for some Hermitian operator H, and for some trainable parameter $\theta \in \mathbb{R}$. In particular, since this must hold for all θ, it must hold for infinitesimal parameters. We can again use the Taylor expansion trick (Eq. (7.29)) to expand around $\theta = 0$. So $e^{-i\theta H} = I - i\theta H + O(\theta^2)$ we get

$$[U(\theta), V_g] = -i\theta[H, V_g] + O(\theta^2), \tag{7.53}$$

which is zero (to first order) if $[H, V_g] = 0$. That is, the quantum neural network $U(\theta)$ will be equivariant if its generator H commutes with all the representations of the group elements. In fact, one can check that

$$[H, V_g] = 0, \quad \forall g \in G, \tag{7.54}$$

is enough to guarantee that all remaining higher orders terms will also commute with V_g. Not surprisingly, it is easier to solve $[H, V_g] = 0$ at the algebra level than to solve $[W(\theta), V_g]$ at the group level.

So for the permutation invariant binary classification problem we were just considering we would need to pick our quantum gates such that all their operators are permutation invariant. That is, we have gates of the form $e^{-i\theta_1 X} \otimes e^{-i\theta_1 X}$ or $e^{-i\theta_2 Z\otimes Z}$. One possible example quantum neural network of this form is shown in Fig. 7.12.

For more examples of how equivariance can be used to design good models (including some more physics inspired ones - e.g. solving ground state problems) see Appendix 7.20.

7.6 (Ir)Reducible Representations of Groups

Our goal here will be discuss when/how it is possible to decompose a representation into a direct sum of other representations and, hopefully, give a sense of why we might be interested in doing this in the first place.

7.6.1 Warm up example

Consider a two qubit system and the tensor product representation of $SU(2)$ on this space, i.e.

$$R(g) = U_g \otimes U_g \,. \tag{7.55}$$

Can we decompose this into the direct sum of two other representations? That is, can we block diagonalize $U_g \otimes U_g$ for all g?

To answer this we first note that $U_g \otimes U_g$ commutes with the SWAP operator $[U_g \otimes U_g, \mathrm{SWAP}] = 0$. This means that it is possible to (block) diagonalize $U_g \otimes U_g$ in the same basis as the SWAP. More generally, the following proposition holds.

Proposition 7.6.1. *Let $R(g) = U_g$ be a representation of a group G, and let H be a Hermitian operator such that $[U_g, H] = 0$ for all $g \in G$. Then, for any eigenvector $|\psi\rangle$ of H with eigenvalue λ, $U_g|\psi\rangle$ is also an eigenvector of H of eigenvalue λ. That is, H is simultaneously block diagonalized with U_g.*

Demo. Observe that $HU_g|\psi\rangle = U_g H|\psi\rangle = \lambda U_g|\psi\rangle$. This means that H and U_g are (block[21]) diagonal in the same basis. ☐

Next we recall that the SWAP operator has eigenvalue 1 on the symmetric subspace spanned by the degenerate eigenstates $\{|11\rangle, |01\rangle + |10\rangle, |00\rangle\}$ and eigenvalue -1 on the anti-symmetric subspace spanned by $\{|10\rangle - |01\rangle\}$. That is, it is block diagonalized in the symmetric-antisymmetric decomposition.

It thus follows that the tensor representation $U_g \otimes U_g$ is also block diagonalized by the symmetric-antisymmetric decomposition of V: i.e., in the basis $\{|11\rangle, |01\rangle + |10\rangle, |00\rangle, |10\rangle - |01\rangle\}$. That is, every representative $U_g \otimes U_g$ can be expressed as

$$U_g \otimes U_g = \left(\begin{array}{ccc|c} & & & 0 \\ & & & 0 \\ & & & 0 \\ \hline 0 & 0 & 0 & \end{array}\right) \tag{7.56}$$

where □ indicates the blocks to be filled in with the appropriate matrix elements. That is, the claim is that if you take any matrix constructed from the tensor product of two single qubit matrices and write it in the Bell basis [22], it will have the block diagonal form shown above [23].

In other words, using the notation $\mathrm{Sym}^2(\mathbb{C}^2)$ for the symmetric subspace and $\mathrm{Alt}^2(\mathbb{C}^2)$ for the antisymmetric subspace, we can write the composite vector space as $V = \mathrm{Sym}^2(\mathbb{C}^2) \oplus \mathrm{Alt}^2(\mathbb{C}^2)$ and it is possible to construct representations that act on these spaces separately. More concretely, it can be built from the direct sum of $SU(1)$ (i.e. just the 1 by 1 identity matrix) on the subspace $\mathrm{Alt}^2(\mathbb{C}^2)$ and $SU(3)$ on the $\mathrm{Sym}^2(\mathbb{C}^2)$ subspace. Note also, that due to the block

[21] The fact we have 'block diagonalized' rather than simply 'diagonalized' here allows for the fact that H and U_g can have degenerate eigenvalues

[22] The subspace spanned by $\{|11\rangle, |01\rangle + |10\rangle, |00\rangle\}$ is alternatively spanned by the Bell states $\{|\Phi^+\rangle, |\Phi^-\rangle, |\Psi^+\rangle\}$.

[23] *Exercise:* If you're not yet fully convinced, check this numerically. It's quite cool to see it work in practise.

structure of $U_g \otimes U_g$ a state in the subspace $\mathrm{Sym}^2(\mathbb{C}^2)$ remains in the subspace spanned by $\mathrm{Sym}^2(\mathbb{C}^2)$ (and similarly for $\mathrm{Alt}^2(\mathbb{C}^2)$).

It is important to stress that it is not always possible to reduce a representation into a direct sum of representations. Or, equivalently, a representation will not always have an invariant subspace. For a simple example of such an *irreducible* representation consider the fundamental representation of $SU(2)$. This is simply the continuous set of all single qubit unitaries. Clearly there is no single basis in which such matrices are all diagonal. Or, equivalently, there is no way to split the vector space into disjoint subspaces where any vector in that space remains in that space under any arbitrary single qubit unitary. Similarly, the representation $SU(2)$ on $\mathrm{Sym}^2(\mathbb{C}^2)$ and $\mathrm{Alt}^2(\mathbb{C}^2)$ cannot be further reduced (e.g. there is no subspace within $\{|11\rangle, |01\rangle+|10\rangle, |00\rangle, |10\rangle-|01\rangle\}$ that remains invariant under any unitary $U \otimes U$ with $U \in SU(2)$).

Before we move on to discussing when representations are and are not reducible let me just highlight that there is lots of physics in the simple example of decomposing $SU(2) \otimes SU(2)$ into a direct sum. And this physics hopefully gives you a sense of why reducing representations is physically interesting.

Link with identical particles. Firstly, thinking back to when we studied identical particles, you should recognise the symmetric and anti-symmetric subspaces found above as corresponding to Bosons and Fermions respectively. Thus these observations could be seen as another way of showing[24] that there are two types of fundamental particles that we cannot transform between.

Link with addition of angular momentum/Clebsch-Gordan coefficients. The two blocks found above also correspond to the spin 1 and spin 0 blocks obtained when adding the momentum of two spin half particles. That is, we have three spin 1 states:

$$|s = 1, m = 1\rangle = |11\rangle \tag{7.57}$$

$$|s = 1, m = 0\rangle = \frac{1}{\sqrt{2}}(|10\rangle + |01\rangle) \tag{7.58}$$

$$|s = 1, m = -1\rangle = |00\rangle \tag{7.59}$$

and one spin 0 state:

$$|s = 0, m = 0\rangle = \frac{1}{\sqrt{2}}(|10\rangle - |01\rangle)\,. \tag{7.60}$$

Here the left hand side of the equations denotes the state corresponding to the total spin $s = s_1+s_2$ of two spin 1/2 particles ($s_1 = 1/2$, $s_2 = 1/2$) and total spin m orientated in the z direction. On the right hand side of the equations we denote the spin orientation of the two particles, e.g. $|10\rangle$ corresponds to one spin aligned spin up with z and the other spin pointing down in the z direction. These equations, read right to left, can be viewed as representing a change in basis from a basis where we list the individual orientations of the spins to the resulting total spin and orientation of the combined spins. Thus we see that the decomposition of a tensor product representation into a direct sum of representation has a deep link with how to add the angular momentum of composite systems.

[24] Technically we just consider the rather trivial $U \otimes U$ evolutions here but the more general set of evolutions that commute with SWAP could similarly be diagonalized in the symmetric and anti-symmetric subspaces.

More generally, when we add two spins j_1 and j_2, we have a spin that can take values j from $j = |j_1 - j_2|$ to $|j_1 + j_2|$. Correspondingly, the tensor product of representation can be decomposed into a direct sum of representations (that cannot themselves be reduced further) corresponding to each of the j values that the composite system can take:

$$D^{j_1} \otimes D^{j_2} = \oplus_{|j_1 - j_2| \le j \le |j_1 + j_2|} D^j \,. \tag{7.61}$$

Here each representation j is of dimension $2j + 1$ (where m takes integer values from $-j$ to j i.e. $m = -j, -j+1, \ldots, j$). This decomposition is often called a Clebsch-Gordan decomposition. The change of basis from the tensor product representation to the direct sum representation corresponds to the change in basis from detailing each particles orientation to detailing the total angular momentum J and orientation M. This change in basis defines the Clebsch-Gordan coefficients:

$$|j, m\rangle = \sum_{m_1=-j_1}^{j_1} \sum_{m_2=-j_2}^{j_2} |j_1, m_1; j_2, m_2\rangle \langle j_1, m_1; j_2, m_2 \mid j, m\rangle \tag{7.62}$$

$$= \sum_{m_1=-j_1}^{j_1} \sum_{m_2=-j_2}^{j_2} C^{J,M}_{j_1,m_1;j_2,m_2} |j_1, m_1; j_2, m_2\rangle \,. \tag{7.63}$$

The theory of groups and irreducible representations can be used to compute this coefficients. However, we won't have time to cover that in detail in this course.

7.6.2 Definitions of (Ir)Reducibility.

Hopefully that example gave you some hint of what we mean by *reducing* representation into a direct sum of representations. Hopefully it also gave you a hint as to why it is physically interesting. I appreciate is right now it might seem like an overkill and all we have done is rephrase ideas from quantum physics 1 in a group theoretic language. However, in more complex scenarios we will start only with the symmetry properties and be faced with the challenge of trying to identify the relevant subspaces. This is when group and representation theory really becomes useful.

Let's define the concepts of reducible and irreducible representations a little more formally.

Definition 7.6.2 (Reducible representation)**.** A representation $R(g)$ of a group G over a vector space V is reducible if there exists an invariant subspace. That is, if there exists a non-trivial (i.e. not just V or $\mathbf{0}$) subspace W of V such that $\forall \, |w\rangle \in W$, we have $R(g)\,|w\rangle \in W$, for any element $g \in G$.

In plain words: an invariant subspace means a smaller space than the actual space V, where the application of any matrix in the representation does not leave the space. In terms of matrices, this means that there is an equivalent representation that can be written as a block matrix with a zero block:

$$R(g) = \begin{pmatrix} Q(g) & 0 \\ T(g) & P(g) \end{pmatrix} \tag{7.64}$$

In fact if we write all vectors in V as $|x\rangle = \begin{pmatrix} v \\ w \end{pmatrix}$, we see that the subspace defined by vectors $|w\rangle = \begin{pmatrix} 0 \\ w \end{pmatrix}$ is transformed as

$$R(g)\,|w\rangle = \begin{pmatrix} 0 \\ P(g)w \end{pmatrix} \tag{7.65}$$

so that such vectors never leave the subspace. If a representation is reducible, then there is a basis such that all matrices can be written as such block matrices in the basis.

Definition 7.6.3 (Irreducible representation)**.** An irreducible representation is a representation that is not reducible.

Obviously, representations that live in dimension 1 are irreducible. One of the main uses of group theory in quantum mechanics is to *reduce* representations into a set of irreducible ones.

A particular case of reducibility is *complete reducibility*, in which case $T(g) = 0$ as well.

Definition 7.6.4 (Completely Reducible representation)**.** A representation $R(g)$ of a group G is completely reducible if it splits into a direct sum of irreducible representations

$$R(g) = \begin{pmatrix} R_1(g) & 0 & \dots & 0 \\ 0 & R_2(g) & \dots & 0 \\ \vdots & & & \\ 0 & 0 & \dots & R_k(g) \end{pmatrix} = \bigoplus_i R_i(g)\,. \tag{7.66}$$

We may wonder if all reducible transformations are completely reducible. Sadly, this is not the case. Here is an example: the matrices

$$M(x) = \begin{pmatrix} 1 & x \\ 0 & 1 \end{pmatrix} \tag{7.67}$$

are a representation of the group $\mathbb{R}, +$. Indeed, $M(x)M(y) = M(x+y)$. However, we cannot diagonalize such matrices.

The good news, however, is that in this lecture we will limit ourselves to *unitary representations* which if they are reducible are always completely reducible[25].

The rest of this chapter will be centred around developing the tools to find and use irreducible representations. More precisely, we are going to do two things: i) Study the consequences of having an irreducible representation, and ii) See how to get an irreducible representation. Irreducible representations are call ‘irreps’ for short. I will sometimes refer to them as such.

A word of warning, the next few sections will get pretty technical. This is unavoidable. If you are ever lost, try and construct yourself some examples of the statements being made. To avoid getting too bogged down in technicalities some of the longer proofs will be left to appendices.

[25]To see this note that since unitary transformation send orthogonal states to orthogonal states $T(g)$ must be zero in equation (7.64).

7.7 How many irreducible representations does a group have?

Let us start by presenting two theorems that can be used to deduce the number of irreps that a group has.

Lemme 7.7.1. *Burnside lemma: For a finite group of order h, there are only a finite number n of irreducible representations $a = 1, \dots, n$ of dimension l_a, and*

$$\sum_{a=1}^{n} l_a^2 = h \tag{7.68}$$

For example, the group $\mathbb{Z}_2$ is order 2 (i.e. contains two elements). It's irreducible representations are the trivial representation, $e \to 1$ and $a \to 1$, and the sign representation, $e \to 1$ and $a \to -1$. And this satisfies the Burnside lemma as $1^2 + 1^2 = 2$. (For a proof of this Theorem see Appendix 7.18).

Lemme 7.7.2. *Number of Irreducible Representations: For a finite group of order h, the number of (non-equivalent) irreps is equal to the number of* ***conjugacy classes****:*

$$N_r = N_c\,. \tag{7.69}$$

To understand this second theorem, which we will prove in Section 7.10, we will need to introduce the concept of a *conjugacy class.*

7.7.1 Equivalence relations and conjugacy classes.

A conjugacy class is a type of equivalence class, which is in turn defined via the notion of an equivalence relation.

Definition 7.7.3 (Equivalence relation)**.** A binary relation $\sim$ on a set X is said to be an equivalence relation, if and only if it is reflexive, symmetric and transitive. That is, for all $a, b, c \in X$, we have:

- $a \sim a$ (*Reflexivity*)
- $a \sim b \Rightarrow b \sim a$ (*Symmetry*)
- $(a \sim b), (b \sim c) \Rightarrow a \sim c$ (Transitivity)

An equivalence relation allows to divide a set into disjoints set called *equivalence classes* as sketched in Fig. 7.13. Of particular importance to us will be *conjugacy classes* (a special type of equivalence class).

Definition 7.7.4 (Conjugacy class)**.** Let G be a group, we define the following equivalence relation: x and y are equivalent if there exists $u \in G$ such that $u^{-1}xu = y$. We then say they belong to the same *conjugacy class.*

Let's verify that the conjugacy class is indeed an equivalence class by showing that the relation defined above satisfies all properties of an equivalence relation.

- Picking $u = x^{-1}$ we have $x^{-1}xx = x$ so that $x \sim x$ (Reflexively).
- If there exists u such that $u^{-1}xu = y$ then $x = uyu^{-1} = (u^{-1})^{-1}yu^{-1}$ so that using $v = u^{-1} \in G$, $\exists v \in G \mid x = v^{-1}yv$. (Symmetry).

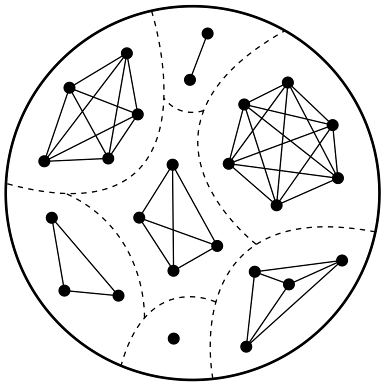


Figure 7.13: Graph of an example equivalence with 7 classes (from Wiki page on equivalence classes).) Each edge represents ~ (with edges from any node to itself not shown).

- if $a \sim b$ and $b \sim c$, then it exists $u, v \in G$ such that $u^{-1}au = b$ and, by symmetry, $v^{-1}cv = b$ so that $u^{-1}au = v^{-1}cv$ and $vu^{-1}auv^{-1} = c$. Using $w = vu^{-1}$ and $w^{-1} = uv^{-1}$ yields $w^{-1}aw = b$. (Transitivity).

Thus the conjugation relation divides the elements of group G into distinct classes which are called conjugate classes or simply classes.

Let us consider for example the order 4 cyclic group:

$$G = \begin{array}{c|cccc} * & e & a & b & c \\ \hline e & e & a & b & c \\ a & a & e & c & b \\ b & b & c & e & a \\ c & c & b & a & e \end{array} \tag{7.70}$$

In this case, can check that we have four conjugacy classes, each containing one member. (But, for example, $\{a, b\}$ is not an equivalence class because there is no $u \in \{a, b\}$ such that $uau^{-1} = b$.)

In fact, this is true for each Abelian group (and the converse is true). An Abelian group of order n has n conjugacy classes. This is a trivial consequence of commutation (i.e. $uau^{-1} = uu^{-1}a = a = b$)! Looking back at Lemma 7.7.2 this then implies that an order n Abelian group has n irreps (irreducible representations).

A more interesting example is given by the C3v group. Here we have three conjugacy classes: $\{e\}$,$\{c_+, c_-\}$, and the three mirrors $\{\sigma, \sigma^{'}, \sigma^{''}\}$ (if you can't see why check out this video). Note that e is always a "isolated" class in itself. Indeed, if $x = u^{-1}eu$ then $x = e$. Looking back at Lemma 7.7.2 this tells us that C3v has 3 irreps.

So we now have a way of counting how many irreps we have. This can be useful because if we are trying to find all irreducible representations of a group because it gives us a way of knowing how many we are missing. Then Burnside's Lemma gives us a way of guessing the dimensions of the missing representations. But this is only so useful. Really we want to know how to identify some of the irreps.

7.8 Schur's lemmas.

A key result to help identify irreps is Schur's lemma. This discusses the link between irreducible representations, and in particular their link with an operator that commutes with all elements of the representation.

Schur's first lemma gives us a criterion to determine when two representations are reducible.

Lemme 7.8.1 (Schur's First Lemma[26]). *Let $R_1(g)$ and $R_2(g)$ be two non-equivalent irreducible representations of a group G, each acting on vector spaces $\mathcal{H}_1$ and $\mathcal{H}_2$:*

$$R_1 : G \to GL(\mathcal{H}_1) \tag{7.71}$$

$$R_2 : G \to GL(\mathcal{H}_2) \tag{7.72}$$

If there is a matrix A is such that

$$AR_1(g) = R_2(g)A \quad \forall g \in G \tag{7.73}$$

then $A = 0$.

Or, turning it around, if you can find an A that satisfies Eq. (7.73) such that $A \neq 0$ then you representations R_1 and R_2 are reducible.

The second lemma studies what kind of matrices commute with all matrices of a given irreducible representation.

Lemme 7.8.2 (Schur's Second Lemma[27]). *Let $R : G \to GL(\mathcal{H}_1)$ be a irreducible unitary representation [28] of a group G. If a matrix A commutes with $R(g)$ for all $g \in G$*

$$AR(g) = R(g)A \quad \forall g \in G,$$

then $A = \lambda I$ for some $\lambda \in \mathbb{C}$. In other words, A is a constant multiple of the identity matrix.

In short, if there exists an operator A that commutes with all elements of two *irreducible* representations then Schur lemmas gives a very strong limit to what A can be: either a trivial diagonal matrix, if the representations are equivalent (i.e., the same up to a change of basis), or a zero one, if they are not. Or, turning it around, no operator - except the trivial zero operator - commutes with all elements of two non-equivalent irreducible representations. So if you find a non-trivial operator that does commute then the representations are reducible.

Example. To make this less abstract let's first consider our favourite example of $SU(2) \otimes SU(2)$. We know that its irreps are $SU(1)$ on the subspace $\mathrm{Alt}^2(\mathbb{C}^2)$ and $SU(3)$ on the subspace $\mathrm{Sym}^2(\mathbb{C}^2)$. It follows from Schur's Second Lemma that the only operators that commute with $SU_3(g)$ on $\mathrm{Sym}^2(\mathbb{C}^2)$ for all g is a scalar multiplication of I on this subspace , i.e. $I = |\Psi^+\rangle\langle\Psi^+| + |\Phi^-\rangle\langle\Phi^-| + |\Phi^+\rangle\langle\Phi^+|$. And this is, of course, indeed the case.

[26] The proof here isn't too bad.

[27] For a nice proof of this check out Group theory in a nutshell for physicists.

[28] For those of you for which these details are important (and/or those who have been confused how Schur's lemma is stated differently in different books/references) the statement and proof of Schur's Second Lemma can differ slightly depending on whether you are looking at finite or infinite dimensional representations. However, we will not worry about these subtleties in this course. It holds in the form stated here for finite or compact unitary representations (i.e. all representations we will be interested in for this course).

As another example of how to apply Schur's lemma let us consider the $R(e) = I$ and $R(a) = X$ representation of Z_2 group. The $A = X \neq I$ operator commutes with both I and X and so we know immediately that $R(e) = I$ and $R(a) = X$ is not an irrep. Note, that this is a consequence of the Z_2 group being Abelian. More generally, from Schur's lemma, we can deduce something very important:

Theorem 7.8.3 (Representation of Abelian groups)**.** *All irreducible representations of Abelian groups are scalar.*

Demo. Let $R(g)$ be an irreducible representation of an Abelian group G. Then we have, $\forall g, h \in G$, $R(g)R(h) = R(g * h) = R(h * g) = R(h)R(g)$. Since $R(h)$ commutes with all $R(g)$, then from the second Schur lemma, it must be a matrix $I\lambda$, and $R(h) = I\lambda(h)$ for all h. Since it is also irreducible, then $R(h) = \lambda(h)$ (i.e. $= I\lambda$ clearly has invariant subspaces for $\dim(I) \geq 2$). □

More generally, given a bunch of matrices, there are potentially many matrices that commute with all of them. However, if the matrices form an irreducible representation of a finite group only multiples of the identity matrix commute with them. In general, we will be interested in problems where the Hamiltonian commutes with a given symmetry of a system. This means that if we can identify the systems irreps we can block diagonalize the Hamiltonian.

Figure 7.14: You may be getting annoyed by now that I promised you theorems to identify irreps but it seems all I've given you are theorems to check if a rep is an irrep. But remember, these theorems also give you constraints on the form the irreps take - which can help you guess them. That said, it's true they do not fully identify them. But be patient. When we get to the orthogonality theorems in a few pages time you'll get some tools that really do help identify them. Credit: L'heure est grave

7.9 Irreps are all about Block Diagonalization!

In a quantum context one often considers the Hamiltonian H, and G a symmetry group that commutes with H. More precisely, if we have a representation of a symmetry group over the Hilbert space $\mathcal{H}$, we have $R(g) : \mathcal{H} \to \mathcal{H}$, and $[R(g), H] = 0 \ \forall \ g \in G$. For example, $\mathcal{H}$ could be an infinite dimensional space, that forms a basis (for instance the Fourier basis). In an infinite dimensional space, we expect that $R(g)$ is reducible. So, if we work hard, we can find a basis of the Hilbert space that reduces the representation, that is we can recompose the space as $\mathcal{H} = \mathcal{H}_1 \oplus \mathcal{H}_2 \oplus \dots$ where all the $\mathcal{H}_i$ are invariant over the group transformation. At this point, we thus have $\forall g \in G, R(g) = R_1(g) \oplus R_2(g) \oplus R_3(g) \dots$ where each of the R_i are irreps, or equivalently in matrix form:

$$R(g) = \begin{pmatrix} R_1(g) & 0 & 0 & \dots \\ 0 & R_2(g) & 0 & \dots \\ 0 & 0 & R_3(g) & \dots \\ \dots \end{pmatrix}. \tag{7.74}$$

In this basis, we write the Hamiltonian (which is of course Hermitian) as

$$H = \begin{pmatrix} H_{11} & H_{12} & H_{13} & \dots \\ H_{21} & H_{22} & H_{23} & \dots \\ H_{31} & H_{32} & H_{33} & \dots \\ \dots \end{pmatrix} = \begin{pmatrix} H_{11} & H_{12} & H_{13} & \dots \\ H_{12}^* & H_{22} & H_{23} & \dots \\ H_{13}^* & H_{23}^* & H_{33} & \dots \\ \dots \end{pmatrix} \tag{7.75}$$

Now, let us see what Schur's lemma tells us. If $[R(g), H] = 0 \ \forall \ g \in G$ then we can apply the Schur lemma between all blocks in this decomposition. Writing out the matrices explicitly, and using $R(g)H = HR(g)$, we see that on the diagonal we have

$$H_{kk} R_k = R_k H_{kk} \tag{7.76}$$

for all k and so by Schur's second lemma along the diagonal we have $\lambda_k I$. Then on the off-diagonal we have terms of the form

$$H_{jk} R_k = R_j H_{jk} \,. \tag{7.77}$$

If R_k and R_j are non-equivalent then, from Schur's first lemma, the block $H_{jk} = 0$. If R_k and R_j are equivalent then the block H_{jk} can be non-zero. That is, assuming only R_1 and R_2 are equivalent, the Hamiltonian can be written as

$$H = \begin{pmatrix} \lambda_1 I & H_{12} & 0 & 0 & \dots \\ H_{21} & \lambda_2 I & 0 & \dots \\ 0 & 0 & \lambda_3 I & 0 & \dots \\ 0 & 0 & 0 & 0 & \dots \\ \dots \end{pmatrix} \tag{7.78}$$

This allows us to considerably simplify the Hamiltonian just from the role of symmetry. In fact, if all the representations are non-equivalent then all the off diagonal terms will have vanished and we have block diagonalized the Hamiltonian - i.e. we know the degenerate eigenspaces of the Hamiltonian. This then makes finding the eigenvalues/eigenvectors of a Hamiltonian much easier as we can just find the eigenvalues/vectors of the individual blocks (which smaller and so easier to handle!) rather than work with the large composite Hamiltonian.

Figure 7.15:

Example for the parity group. A parity transformation (also called parity inversion) is the flip in the sign of a spatial coordinate. In three dimensions, it refers to the simultaneous flip in the sign of all three spatial coordinates (a point reflection): $\mathbf{P}:\begin{pmatrix}x\\y\\z\end{pmatrix}\mapsto\begin{pmatrix}-x\\-y\\-z\end{pmatrix}$. A wave function can always be decomposed into an even and an odd component $\psi(\boldsymbol{x})=\psi^+(\boldsymbol{x})+\psi^-(\boldsymbol{x})$, and the application of the parity operator transforms it as

$$\mathbf{P}\psi(\boldsymbol{x})=\mathbf{P}\psi^+(\boldsymbol{x})+\mathbf{P}\psi^-(\boldsymbol{x})=\psi^+(-\boldsymbol{x})+\psi^-(-\boldsymbol{x})=\psi^+(\boldsymbol{x})-\psi^-(\boldsymbol{x}) \tag{7.79}$$

Note in particular that $\mathbf{PP}=1$. The set of all parity transformations that can be obtained by the parity operator is thus limited to 2. The set of of these transformations forms the parity group $Z_2=\{e,p\}$ that has the following Cayley table:

	e	p
e	e	p
p	p	e

We recall that from Lemma 7.7.2 and the fact that Abelian groups of order n have n conjugacy classes, that this group has only two possible irreducible representations in dimension 1 on $\mathbb{R}$: (i) $R_1(e)=1$ and $R(p)=1$ and (ii) $R_2(e)=1, R_2(p)=-1$.

Consider now a problem with a Hamiltonian that commutes with any parity transformation. The Hamiltonian lives in a large (possibly infinite) Hilbert space $\mathcal{H}$. Now, we consider a basis of $\mathcal{H}$ made of even and odd functions (such as the Fourier basis): $\{\phi_1^+(x),\phi_2^+(x),\ldots,\phi_1^-(x),\phi_2^-(x),\ldots\}$.

This basis defines invariant subspaces with respect to parity, i.e. for any possible representation R of the parity group, even (odd) basis function stays even (odd) under any application of $R(e)$ or $R(p)$. We can therefore use this basis to decompose the Hamiltonian into irreducible representations of $R(e)$ and $R(p)$ as

$$R(e) = \begin{pmatrix} 1 & 0 & 0 & 0 & \dots \\ 0 & 1 & 0 & 0 & \dots \\ 0 & 0 & 1 & 0 & \dots \\ 0 & 0 & 0 & 1 & \dots \\ \dots \end{pmatrix} \text{ and } R(p) = \begin{pmatrix} 1 & 0 & 0 & 0 & \dots \\ 0 & 1 & 0 & 0 & \dots \\ \dots \\ \dots & \dots & -1 & 0 & 0 \\ \dots & \dots & 0 & -1 & 0 \\ \dots \end{pmatrix}$$

where in $R(p)$ the rows/columns with $+1$ correspond to even basis states and the rows/columns with -1 correspond to the odd basis states. That is, we have

$$R(g) = \begin{pmatrix} R_1(g) & 0 & 0 & 0 & \dots \\ 0 & R_1(g) & 0 & 0 & \dots \\ \dots \\ 0 & 0 & R_2(g) & 0 & \dots \\ 0 & 0 & 0 & R_2(g) & \dots \\ \dots \end{pmatrix}. \tag{7.80}$$

Applying the Schur lemmas, and noting that $R_1(g)$ and $R_2(g)$ are non-equivalent irreps, we now obtain that

$$H = \begin{pmatrix} H_{11} & 0 \\ 0 & H_{22} \end{pmatrix}. \tag{7.81}$$

7.10 Orthogonality theorems

We have just seen that if we know a systems irreps we can use them to block diagonalize a Hamiltonian. But we still don't have all the theoretical tools we need to identify irreps in the first place. We will set some of these out in this subsection.

7.10.1 Grand Orthogonality Theorem

We are now in a position to state the grand orthogonality theorem. Similarly to how the orthogonality of eigenstates of a Hermitian operator allows you to find a single eigenstate and then identify other eigenstates by construction, we will see that this theorem allows us to take one irrep and identify others by this orthogonality constraint.

We can think of irreducible representations as giving "vectors of matrices" $([R(g)]_{ij})_{g\in G}$ in a vector space of dimension $|G|$. The Grand Orthogonality Theorem provides orthogonality relations between these vectors. Let me start by stating the theorem in its full glory:

Theorem 7.10.1 (Grand Orthogonality Theorem)**.** *Let R_a and R_b be two non-equivalent unitary irreducible representations of a finite[29] group G of order N. Let n_a and n_b be the dimensions of the vector space for R_a and R_b. Then the grand orthogonality theorem states that*

$$\sum_{g\in G} \frac{n_a}{N} \left[R_a(g)^\dagger\right]_{jk} \left[R_b(g)\right]_{lm} = \delta_{ab}\delta_{jm}\delta_{lk} \tag{7.82}$$

The grand orthogonality theorem is a consequence of Schur's lemma, for a derivation see Appendix 7.17.

Now let me try and unpick it a little for you. Let's first consider the case of two non-equivalent irreps (i.e, $a \neq b$). Then the grand orthogonality theorem implies that the vectors of matrices corresponding to any two non-equivalent irreps are orthogonal[30]. In particular, we have

$$\sum_{g\in G} \left[R_a(g)^\dagger\right]_{jk} \left[R_b(g)\right]_{lm} = 0, \forall \ \ a \neq b\,, \forall i,j,k,l\,. \tag{7.83}$$

Next let's consider the case where $a = b$ so that we're just looking at the properties of a single irrep. In this case we firstly have an orthogonality relation between the elements of the irreps

$$\sum_{g\in G} \left[R_a(g)^\dagger\right]_{jk} \left[R_a(g)\right]_{lm} = 0 \text{ if } j \neq m \text{ and/or } l \neq k\,. \tag{7.84}$$

Finally, the grand orthogonality theorem provides a normalisation condition for these vectors in the case where $j = m$ and $l = k$. Concretely, we have

$$\sum_{g\in G} \left[R_a(g)^*\right]_{kj} \left[R_a(g)\right]_{kj} = \frac{N}{n_a}\,. \tag{7.85}$$

where N is the order of group G and n_a is the dimension of the vector space of representation R_a.

[29] The theorem can also be generalized to compact Lie groups.

[30] Note, that in fact the condition the Grand Orthogonality Theorem imposes is stronger than simply the orthogonality of these vectors. That would be the claim that $\sum_g R_a(g)^\dagger R_b(g) = 0$ which is equivalent to $\sum_g \sum_j [R_a(g)^\dagger]_{ij}[R_b(g)]_{jk} = 0$ for all i and k. This is implied by Eq.(7.83) but Eq.(7.83) is stronger.

Examples. As ever, let us try and make this a little less abstract by considering some examples. Let us start with the Z_2 group. It is Abelian so its irreps are one-dimensional. Specifically, we have:

$$R_1(e) = 1, R_1(a) = 1 \tag{7.86}$$
$$R_2(e) = 1, R_2(a) = -1\,. \tag{7.87}$$

As these are one-dimensional irreps we can drop the subscripts j, k, l, m in Eq. (7.83) and have:

$$\sum_g R_1(g)^\dagger R_2(g) = R_1(e)^\dagger R_2(e) + R_1(a)^\dagger R_2(a) = 1 \times 1 + 1 \times (-1) = 0 \tag{7.88}$$

in agreement with Eq. (7.83). Similarly,

$$\begin{aligned}\sum_g R_1(g)^\dagger R_1(g) &= 1 \times 1 + 1 \times 1 = 2\\ \sum_g R_2(g)^\dagger R_2(g) &= 1 \times 1 + -1 \times (-1) = 2\,.\end{aligned} \tag{7.89}$$

As the order of the group is 2 ($N = 2$) and the dimension of the irreps are 1 ($n_A = 1$) this agrees with Eq. (7.85).

As a less trivial example, let's consider C3v. Remember, this consisting of two rotations (clockwise and anti-clockwise) and three reflections (on each axis). A possible irreducible representation [31] are the following six real matrices:

$$\begin{aligned}
&e = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\\
&c_+ = \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}, \; c_- = \begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}\\
&\sigma = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}, \; \sigma' = \begin{pmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}, \; \sigma'' = \begin{pmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}
\end{aligned} \tag{7.90}$$

Let us consider an example of the normalisation condition first:

$$\sum_{g \in G} R^\dagger(g)_{11} R(g)_{11} = 1^2 + 1^2 + \left(-\frac{1}{2}\right)^2 + \left(-\frac{1}{2}\right)^2 + \left(-\frac{1}{2}\right)^2 + \left(-\frac{1}{2}\right)^2 = 3 = \frac{6}{2}.$$

which satisfies Eq. (7.85) as the order of the group is 6 ($N = 6$) and the dimension of the irrep is 2 ($n_A = 2$). Now let's demonstrate the orthogonality of the $(1,1)$ and $(2,2)$ elements:

$$\sum_{g \in G} R(g)^\dagger_{11} R(g)_{22} = 1^2 + (1)(-1) + \left(-\frac{1}{2}\right)\frac{1}{2} + \left(-\frac{1}{2}\right)\left(-\frac{1}{2}\right) + \left(-\frac{1}{2}\right)\left(-\frac{1}{2}\right) + \left(-\frac{1}{2}\right)\frac{1}{2} = 0.$$

It is straightforward to verify the orthogonality of the other elements.

A direct consequence of the grand orthogonality theorem is that

Proposition 7.10.2. *A finite group can only have a finite number of inequivalent irreducible representations. Specifically, the maximum number of possible irreps is given by the order of the group.*

This is clear from the orthogonality theorem. Thinking of irreducible representations as giving "vectors of matrices" $([R(g)]_{ij})_{g \in G}$ in a vector space of dimension $|G|$, the theorem tells us that those vectors must be orthogonal. But there are at most $|G|$ orthogonal vectors in a vector space of dimension $|G|$, and so the number of irreducible representations must be finite. In fact, we will calculate the number of irreducible representations for any finite group explicitly when we introduce characters.

[31] We will discuss how to check that this is indeed an irrep and discuss other irreps of C3v in Section 7.11.1

7.10.2 Group averaging (twirling)

You may have noticed that the grand orthogonality theorem looks a lot like an average of an object under the adjoint action of the group. To see this consider the quantity:

$$\langle X \rangle_G := \frac{1}{N} \sum_g R(g) X R(g)^\dagger . \tag{7.91}$$

For example, if $R(g) = U_g$ is a unitary representation then this is just the average output of X after being evolved by each unitary U_g in the group,

$$\langle X \rangle_G := \frac{1}{N} \sum_g U_g X U_g^\dagger . \tag{7.92}$$

If this representation is irreducible then we can apply the grand orthogonality theorem to get the following **Irrep Group Averaging Corollary**:

$$\begin{aligned} \langle X \rangle_G &= \frac{1}{N} \sum_{jklm} \sum_g [R(g)]_{lm} X_{mj} [R(g)^\dagger]_{jk} |l\rangle\langle k| \\ &= \frac{1}{d} \sum_{jklm} \delta_{lk} \delta_{jm} X_{mj} |l\rangle\langle k| \\ &= \frac{1}{d} \sum_{jk} X_{jj} |k\rangle\langle k| \\ &= \frac{1}{d} \mathrm{Tr}[X]\, I \end{aligned} \tag{7.93}$$

where $n_a = d$ is the dimension of the vector space of the representation.

Let's consider the group average of the single qubit Pauli group $G = \{\pm(i)\sigma_x, \pm(i)\sigma_y, \pm(i)\sigma_z, \pm(i)I\}$ over an arbitrary single qubit initial state ρ. This is an irreducible representation onto a $d = 2$ vector space and so from Eq. (7.93) we should have

$$\langle \rho \rangle_G = \frac{I}{2} . \tag{7.94}$$

That is, averaging the effect of applying each of the Paulis on a given state gives a maximally mixed state.

If it helps to make this less abstract and mysterious we can also compute $\langle \rho \rangle_G$ explicitly. To do so we first note that in each term of the form $U_g \rho U_g^\dagger$ the +1, -1, $+i$, $-i$ signs cancel out, i.e. $(i\sigma_z)\rho(-i\sigma_z) = \sigma_z \rho \sigma_z$, and so we can write

$$\langle \rho \rangle_G = \frac{1}{4} (\sigma_x \rho \sigma_x + \sigma_y \rho \sigma_y + \sigma_z \rho \sigma_z + I \rho I) . \tag{7.95}$$

If we write the state in terms of its Bloch vector, $\rho = \frac{1}{2}(I + \boldsymbol{r}.\boldsymbol{\sigma})$ and remember the properties of Pauli matrices (e.g. $\sigma_i \sigma_j \sigma_i = -\sigma_j$ for $i \neq j$ but $\sigma_j^3 = \sigma_j$) then we have

$$\langle \rho \rangle_G = \frac{1}{2} \left(I + \frac{1}{4} \left(\begin{pmatrix} r_x \\ -r_y \\ -r_z \end{pmatrix} + \begin{pmatrix} -r_x \\ r_y \\ -r_z \end{pmatrix} + \begin{pmatrix} -r_x \\ -r_y \\ r_z \end{pmatrix} + \begin{pmatrix} r_x \\ r_y \\ r_z \end{pmatrix} \right) . \boldsymbol{\sigma} \right) = \frac{1}{2} I , \tag{7.96}$$

in agreement with Eq. (7.94)

All this discussion of orthogonality theorems so far (i.e., both the grand orthogonality theorem and the group averaging corollary) has been framed for finite groups; however, it also carries over to compact (i.e. closed and bounded) Lie groups. And all the continuous groups we normally care about $U(n)$, $SU(n)$, $O(n)$, $SO(n)$ etc are compact. In this case the finite average sum $\frac{1}{N}\sum_g$ becomes a continuous integral over a uniform measure $\int d\mu(g)$. This uniform measure is called the Haar measure and the average is called Haar averaging - it's exact form and properties are beyond this course but I highly recommend this blog or this review. In any case, for continuous groups the average over irreducible representations is given by:

$$\langle X\rangle_G := \int_G d\mu(g) U_x(g) X U_x(g)^\dagger = \frac{1}{d}\,\mathrm{Tr}[X]\,I\,. \tag{7.97}$$

The operator $\int_G d\mu(g) U_x(g) ... U_x(g)^\dagger$ is sometimes called the *twirling* operation[32].

For example, if you apply random unitaries to a single qubit state and then average the states you get out you will end up with the maximally mixed state. Note you effectively saw this in the decoherence problem sheet - but then I was nice and made the calculation simpler and had you just average over a mix of rotations around the σ_z and σ_x axes rather than arbitrary unitaries.

If you think back to the decoherence problem sheet you'll remember that if you only averaged over $R_z(\theta) = e^{-i\theta\sigma_z}$ rotations then you ended up not at the maximally mixed state but on projecting the state onto the Z axis. How can we understand this?

The first thing to note is that we cannot directly apply Eq. (7.97) because that only holds for irreps and $R_z(\theta) = e^{-i\theta\sigma_z}$ is not an irrep. To see this note that here we are considering U(1) which is an Abelian group and so all its irreps are 1D. So we need a generalization of Eq. (7.97) for reducible representations.

Any reducible unitary representation can be written in the form

$$U(g) = \bigoplus_x U_x(g) = \sum_x U_x(g) \otimes I_{\bar{x}} \tag{7.98}$$

where $\bar{x}$ denotes the subspace that U_x does not act on. Let us repeat the calculation in Eq. (7.93) but this consider a reducible representation written as in Eq. (7.98). Again we'll do this calculation for a finite group but it generalises to continuous groups. Thus if we use the grand orthogonality theorem to repeat the calculation in Eq. (7.93) we find:

$$\begin{aligned}
\langle X\rangle_G &= \frac{1}{N}\sum_g U(g) X U(g)^\dagger \\
&= \frac{1}{N}\sum_g \sum_{xx'} (U_x(g)\otimes I_{\bar{x}}) X (U_{x'}(g)^\dagger \otimes I_{\bar{x}}) \\
&= \frac{1}{N}\sum_g \sum_{x} (U_x(g)\otimes I_{\bar{x}}) X (U_{x}(g)^\dagger \otimes I_{\bar{x}}) \\
&= \frac{1}{d_x}\sum_x \mathrm{Tr}[X\Pi_x]\Pi_x \otimes I_{\bar{x}} \\
&= \frac{1}{d_x}\bigoplus_x \mathrm{Tr}[X\Pi_x]\Pi_x
\end{aligned} \tag{7.99}$$

where Π_x denotes the identity projector onto the subspace spanned by the representation. That is, the input is projected down onto the irreps. (As a sanity check note that if we are actually looking at an irrep then we have $\Pi_x = I$ and $\mathrm{Tr}_x = \mathrm{Tr}$ and so Eq. (7.99) reduces to Eq. (7.93)).

[32] In a quantum information context it is such standard terminology that I thought everyone called it this. However, apparently not... which lead to a few awkward conversations before I realised this.

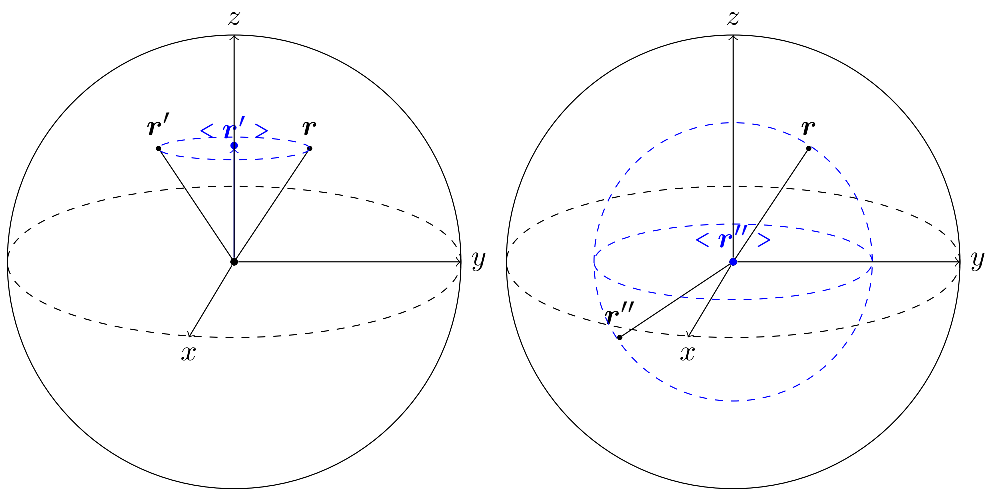


Figure 7.16: Left: We want the average of state $\rho = \frac{1}{2}(\mathbb{1} + \boldsymbol{r}\cdot\boldsymbol{\sigma})$ by $R_z(\theta)$ where $\boldsymbol{r} = (r_x, r_y, r_z)$. If we rotate ρ around the z-axis it goes to $\rho' = \frac{1}{2}(\mathbb{1} + \boldsymbol{r}'\cdot\boldsymbol{\sigma})$ where $\boldsymbol{r}' = (r'_x, r'_y, r_z)$. So if we calculate the average it would be a density matrix with a vector in the Block sphere equal to $(0, 0, r_z)$ which is along the z-axis. Right: And when we have all Pauli matrices, it will be an arbitrary rotation. So the state $\rho = \frac{1}{2}(\mathbb{1} + \boldsymbol{r}\cdot\boldsymbol{\sigma})$ rotates and goes to $\rho'' = \frac{1}{2}(\mathbb{1} + \boldsymbol{r}''\cdot\boldsymbol{\sigma})$ where $\boldsymbol{r}'' = (r''_x, r''_y, r''_z)$ is another arbitrary vector. Then the average is a density matrix with vector zero in the Block sphere.

Again, while I have worked through this calculation for a finite group it also carries over to averaging over all the standard continuous groups we are interested in.

Ok so what happens when we average a state ρ by $R_z(\theta) = e^{-i\theta\sigma_z}$? Well the relevant group here is $U(1)$ and so the irreps in this case are both 1D ($\{1\}$ and $\{e^{-i\theta\theta}\}$) and we have:

$$U_g == \begin{pmatrix} 1 & 0 \\ 0 & e^{-i\theta} \end{pmatrix} = |0\rangle\langle 0| + e^{-i\theta}|1\rangle\langle 1| \tag{7.100}$$

such that $\Pi_0 = |0\rangle\langle 0|$ and $\Pi_1 = |1\rangle\langle 1|$

$$\langle\rho\rangle_G = \frac{1}{1}\bigoplus_{x=0,1} \mathrm{Tr}[\rho\Pi_x]\Pi_x = \langle 0|\rho|0\rangle|0\rangle\langle 0| + \langle 1|\rho|1\rangle|1\rangle\langle 1|\,. \tag{7.101}$$

Thus as we expected (inline with Problem Sheet 5) this averaging kills off all coherence and projects onto the Z axis. For a visualisation of the effect of twirling on the Bloch sphere see Fig. 7.16.

Exercise: What happens if you twirl a qubit state over the group $SU(2) \otimes SU(2)$?

7.10.3 Petit Orthogonality Theorem.

We just saw that the grand orthogonality theorem is effectively an orthogonality relation between "vectors of matrices" $([R(g)]_{ij})_{g\in G}$. We will now consider the petite orthogonality theorem, its simpler corollary, which is an orthogonality relation between vectors composed of their traces $(\chi_R(g))_{g\in G}$ where we have defined

$$\chi_R(g) := \mathrm{Tr}[R(g)]\,. \tag{7.102}$$

We further note that $\mathrm{Tr}(R(x)^\dagger) = \chi_R^*(x)$.

Figure 7.17: **Motivational cat.** Here's also a link to one of my favourite cat videos. It's an old one, and a slow burner (from an era pre-tiktok when videos could be more than 60 seconds), but I think it's one of the best.

Theorem 7.10.3 (Classes & Traces)**.** *In a representation R, all the elements which are in the same conjugacy class have the same trace.*

Demo. If there exists u such that $x = u^{-1}yu$ then

$$\begin{aligned}\mathrm{Tr}(R(x)) &= \mathrm{Tr}(R(u^{-1}yu)) = \mathrm{Tr}(R(u^{-1})R(y)R(u)) = \mathrm{Tr}(R(u)R(u^{-1})R(y)) = \mathrm{Tr}(R(e)R(y)) \\ &= \mathrm{Tr}(R(y))\end{aligned} \tag{7.103}$$

□

From the Grand Orthogonality Theorem, we find

$$\sum_{jk}\sum_{g\in G}\frac{n_a}{N}\left[R_a(g)^\dagger\right]_{jj}\left[R_b(g)\right]_{kk} = \sum_{g\in G}\frac{n_a}{N}\chi_a^*(g)\chi_b(g) = \delta_{ab}\sum_{jk}\delta_{jk}\delta_{jk} = n_a\delta_{ab} \tag{7.104}$$

where in the final line we use the fact that $\sum_{j,k=1}^{n_A}\delta_{j,k}\delta_{jk} = \sum_{j,k=1}^{n_A}\delta_{jk} = n_a$. Thus we see that the vectors of traces of two irreps are orthogonal. Or more formally:

Theorem 7.10.4 (Petit Orthogonality Theorem)**.** *Let R_a and R_b denote two non-equivalent unitary irreducible representations of a finite group of order N, we have*

$$\sum_{g\in G}\chi_a^*(g)\chi_b(g) = N\delta_{a,b} \tag{7.105}$$

As elements in a conjugacy class have the same trace, one can equivalently write the petit orthogonality theorem by summing over the number of the conjugacy classes, i.e. we have

$$\sum_{\mu=1}^{N_c} n_\mu\chi_a^*(C_\mu)\chi_b(C_\mu) = N\delta_{a,b} \tag{7.106}$$

where n_μ denotes the number of elements in class μ and N_c is the total number of conjugacy classes.

For example, in the case of C3v we have three equivalent classes: $\{e\}$,$\{c_+, c_-\}$, and the three mirrors $\{\sigma, \sigma^{'}, ^{\sigma''}\}$. We see in Eq. (7.90) that $\chi(e) = 2$, $\chi(c_+) = \chi(c_-) = -1$ and $\chi(\sigma) = \chi(\sigma^{'}) =$

$\chi(\sigma'') = 0$. Thus, in line with Eq. (7.106), we have $1 \times 2^2 + 2 \times (-1)^2 + 3 \times 0^2 = 6$.

We stress that we can interpret this theorem as an orthogonality relation of N_r (the number of representations) vectors in a space of dimension N_c (the number of equivalent classes). Indeed, for any representation a we can define the (N_c-dimensional) vectors:

$$[|a\rangle]_\mu = \sqrt{\frac{n_\mu}{N}} \chi_a(C_\mu) \quad \text{for } \mu = 1, ..., N_c \,. \tag{7.107}$$

There are N_r of these vectors for the N_r different irreps. It follows from Eq. (7.106) that this set of N_r vectors are all orthogonal. Since the maximum numbers of orthogonal vectors is N_c, we have

$$N_r \leq N_c \,. \tag{7.108}$$

That is, the number of representation is smaller or equal to the number of conjugation classes. This is the first step towards proving Lemma 7.7.2 (i.e. that the number of irreps is equal to the number of conjugacy classes) which we stated without proof earlier. In turns out this bound is tight (this is another consequence of the Grand Orthogonality Theorem - for a proof see Vincenzo Savona's notes on page 37) leading to Lemma 7.7.2.

Figure 7.18: **Motivational Panda.** Even if you're struggling a little to follow by this point you're still doing better than this panda. (God knows how these animals survive in the wild).

Again, that was quite lot of quite technical material. And we've got more to come. So here's a panda. And if fluffy animals aren't your thing here's a clip of two guys trying to kayak down a melting ski slope.

7.11 Characters

We saw above that the traces of a representation of a group are useful. The set of traces associated with a representation are known as the *character* of the representation. Characters provide an elegant and systematic approach to analyzing and categorizing irreducible representations, as well as ascertaining the reducibility of a specific representation.

Definition 7.11.1 (Character)**.** The set of all traces $\{\chi_R(g)\}$ is called the character of the representation R.

As we saw above, two equivalent representations have the same character. Indeed if $R_2(g) = SR_1(g)S^{-1}$, then using the cyclic property of the trace we have $\mathrm{Tr}[R_2(g)] = \mathrm{Tr}[SR_1(g)S^{-1}] = \mathrm{Tr}[R_1(g)]$. In fact this is a sufficient condition as well:

Theorem 7.11.2 (Characters of Irreps)**.** *Two irreps are equivalent if and only if they have the same character.*

Demo. We already proved that the condition is necessary. To prove it is sufficient we reason by contradiction. Assume two irreps R_1 and R_2 are not equivalent but have the same character. Then using the petit Orthogonality theorem, we find that the sum of (modulus of) trace squared should be zero, which is impossible as the norm squared is positive and non-zero (the identity conjugacy class has trace 1). □

Or, turning it around, different (non-equivalent) irreps have different characters.

Using this approach, we can now compute degeneracy numbers for representations, that is compute how many copies of an irrep a given reducible representation contains. We first write:

$$R(g) = R_{1,1}(g) \oplus R_{1,2}(g) ... \oplus R_{1,b_1}(g) \oplus R_{2,1}(g) \oplus R_{2,2}(g) ... \oplus R_{2,b_2}(g) ... = \oplus_{a,x} R_{a,x}(g) \quad (7.109)$$

where $x = 1, ..., b_a$ with b_a denoting the degeneracy number. The question is how to find b_a? Using the characters of each irreps, we know that:

$$\chi_R(g) = \mathrm{Tr}\left[\begin{pmatrix} R_{1,1}(g) & 0 & 0 & 0 & \dots \\ 0 & ... & 0 & 0 & \dots \\ 0 & 0 & R_{1,b_1}(g) & 0 & \dots \\ 0 & 0 & 0 & R_{2,1}(g) & \dots \\ \dots & & & & \end{pmatrix}\right] = \sum_i b_a \mathrm{Tr}[R_a(g)] = \sum_a b_a \chi_a(g)\,. \quad (7.110)$$

As the trace of all representations within the same conjugacy class are the same we can equivalently write

$$\chi_R(C_\mu) = \sum_a b_a \chi_a(C_\mu)\,. \quad (7.111)$$

We can combine this expression with the petite orthogonal theorem to find an expression for b_a. To do so we multiply by $n_\mu \chi_b^*(C_\mu)$, where n_μ is the number of element in class C_μ, and sum over classes

$$\sum_{\mu=1}^{N_c} n_\mu \chi_b^*(C_\mu)\chi_R(C_\mu) = \sum_{\mu=1}^{N_c} n_\mu \sum_a b_a \chi_b^*(C_\mu)\chi_a(C_\mu) \quad (7.112)$$

$$= \sum_a b_a \sum_{\mu=1}^{N_c} n_\mu \chi_b^*(C_\mu)\chi_a(C_\mu) = \sum_a b_a N \delta_{a,b} = N b_b \quad (7.113)$$

so that

$$b_a = \frac{1}{N}\sum_{\mu=1}^{N_c} n_\mu \chi_a^*(C_\mu)\chi_R(C_\mu) = \frac{1}{N}\sum_{\mu=1}^{N_c} n_\mu \chi_a^*(C_\mu)\chi_R(C_\mu)\,. \quad (7.114)$$

We thus now have a formula for each number of irreps contained in a given representation:

Theorem 7.11.3 (Computing Degeneracy)**.** *Assume a decomposition in irreps as*

$$R(g) = \oplus_{a,x} R_{a,x}(g) \quad (7.115)$$

for $x = 1, ..., b_a$. Then we have

$$b_a = \frac{1}{N}\sum_\mu n_\mu \chi_a^*(C_\mu)\chi_R(C_\mu) \quad (7.116)$$

Remember this formula! It will be very useful in the problem sheets this week.

Another interesting consequence of the petite orthogonal theorem is the following one:

Theorem 7.11.4 (Sufficient condition for irreps)**.** *A necessary and sufficient condition for a representation R to be an irrep is that*

$$\sum_{\mu=1}^{N_c} n_\mu |\chi(C_\mu)|^2 = N \quad (7.117)$$

Demo. Using Eq.(7.111) and the petit orthogonality theorem (Eq.(7.106)), we find that

$$\sum_{\mu=1}^{N_c} n_\mu |\chi(C_\mu)|^2 = \sum_{i,j} b_i b_j \sum_{\mu=1}^{N_c} n_\mu \chi_i(C_\mu)^* \chi_j(C_\mu) = N\sum_{i,j} b_i b_j \delta_{ij} = N \sum_i b_i^2 \quad (7.118)$$

Being irreducible means having only one of the b_i=1, which proves the theorem. □

For a finite group, it is easy to find the characters listed in table in the literature (google is your friend!), listed as follows:

irrep\ class	$C_1(e)$	C_2	C_3	C_4	C_5
R_1	1	1	1	1	1
R_2	d_2	$\chi_2(C_2)$	$\chi_2(C_3)$	$\chi_2(C_4)$	$\chi_2(C_5)$
R_3	d_3	$\chi_3(C_2)$	$\chi_3(C_3)$	$\chi_3(C_4)$	$\chi_3(C_5)$
R_4	d_4	$\chi_4(C_2)$	$\chi_4(C_3)$	$\chi_4(C_4)$	$\chi_4(C_5)$
R_5	d_5	$\chi_5(C_2)$	$\chi_5(C_3)$	$\chi_5(C_4)$	$\chi_5(C_5)$

7.11.1 Example with C3v.

Ok we now finally have the tools to put everything together and show how orthogonality relations can be used to identify irreps.

Let us again consider the C3v group, i.e. symmetry of the triangle. We first recall that it is a non-Abelian group of order 6. The conjugacy classes are $C_e = \{e\}, C_1 = \{c_+, c_-\}$ and $C_2 = \{\sigma, \sigma', \sigma''\}$ and so, as we saw before, from Lemma (7.7.2) there can be only 3 irreps.

We saw the 2D irrep in Eq. (7.90):

$$\begin{aligned} R(e) &= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \\ R(c_+) &= \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}, R(c_-) = \begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix} \\ R(\sigma) &= \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}, R(\sigma') = \begin{pmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}, R(\sigma'') = \begin{pmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix} \end{aligned} \tag{7.119}$$

There we simply claimed that this was an irrep. Now we can use Theorem 7.11.4 to check. Namely we have,

$$\sum_{\mu=1}^{N_c} n_\mu |\chi(C_\mu)|^2 = 1 \times 2^2 + 2 \times (-1)^2 + 3 \times 0 = 6 = N\,. \tag{7.120}$$

What are the other irreps? We can of course have the trivial irrep where every group element is represented by a scalar equal to one. The trivial 1D irrep:

$$R(e) = 1, R(c_+) = 1, R(c_-) = 1, R(\sigma) = 1, R(\sigma') = 1, R(\sigma'') = 1 \tag{7.121}$$

(This is indeed an irreducible representation as $1 + 2 \times 1 + 3 \times 1 = 6$ in line with Theorem 7.11.4).

Now to identify the missing irrep. From Burnside's Lemma we know that it has to be 1D (i.e, $1^2 + 2^2 + l^2 = 6$ implies $l = 1$). From the petit orthogonality theorem we know that the characters of this final representation must be orthogonal. Thus denote the characters of the missing representation as $(\chi_e, \chi_c, \chi_c, \chi_\sigma, \chi_\sigma, \chi_\sigma)$ we have $(1, 1, 1, 1, 1, 1).(\chi_e, \chi_c, \chi_c, \chi_\sigma, \chi_\sigma, \chi_\sigma) = \chi_e + 2\chi_c + 3\chi_\sigma = 0$ and $(2, -1, -1, 0, 0, 0).(\chi_e, \chi_c, \chi_c, \chi_\sigma, \chi_\sigma, \chi_\sigma) = 2\chi_e - 2\chi_c = 0$. Thus we have $\chi_e = \chi_c$ and $\chi_\sigma = -\chi_e$. The only 1D representation that satisfies these conditions and Lemma (7.7.2) is thus:

$$R(e) = 1, R(c_+) = 1, R(c_-) = 1, R(\sigma) = -1, R(\sigma') = -1, R(\sigma'') = -1 \tag{7.122}$$

(Check for yourself that this is indeed an irrep for C3v!)

Thus for the character table for the group C3v we have Table 7.13.

	e	$2C_3$	$3\sigma_v$
A_1	1	1	1
A_2	1	1	-1
E	2	-1	0

Table 7.1: Character table for point group C3v. Here $A1$ and $A2$ deontes the 1D representation in Eq. (7.121) and Eq. (7.122), and E denotes the $2D$ representation in Eq.(7.90).

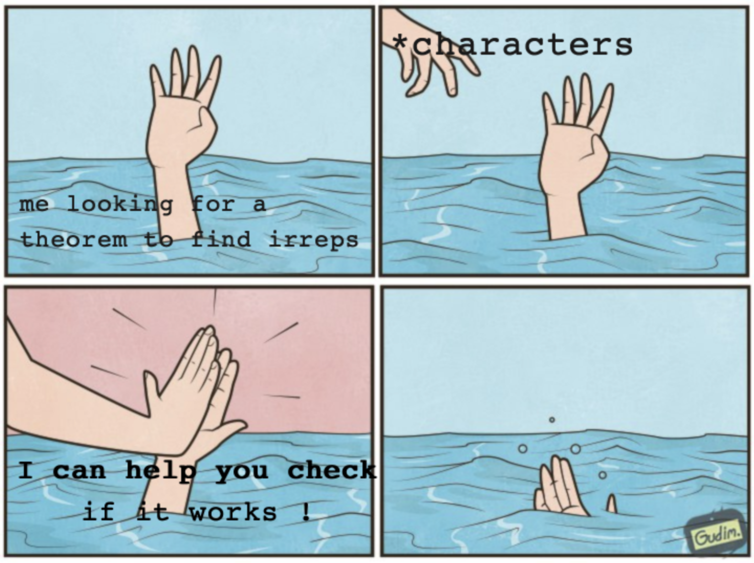


Figure 7.19: Note that in the above example we could get away with just studying the characters and the petite orthogonality theorem to identify our irreps. However, in general the characters will not suffice and you'll have to have already identified some non-trivial irreps and then can use the grand orthogonality theorem to help you identify the remainders. That said, even in this case knowing the character at least helps you guess the diagonal of your irrep. Credit: Mehdi Haddad.

7.12 Projectors

In the last section and in the problems for last week you saw how to reduce a representation into a direct sum of irreducible representations. (For example, in Problem 2 we saw how a 3D representation of C3v could be written as a direct sum of the groups 2D and 1D irreps). In general, Theorem 7.11.3 allows us to compute how many times any irrep appears in any representation we are trying to reduce. But we have yet to establish a general strategy for finding the *basis* in which the representation is block diagonalized to the sum of irreps. We address that in this section.

7.12.1 Basis notation

Let us start by introducing *basis notation.* As we saw in the previous section, we can take a representation and write it as a direct sum of irreducible representations. That is, we can write $R(g) = \oplus_{a,x} R(a, x(g))$, or equivalently

$$R(g) = \begin{pmatrix} R_1(g) & 0 & 0 & 0 & \dots \\ 0 & R_1(g) & 0 & 0 & \dots \\ 0 & 0 & R_2(g) & 0 & \dots \\ 0 & 0 & 0 & R_2(g) & \dots \\ \dots & & & & \end{pmatrix} = \begin{pmatrix} R_{1,1}(g) & 0 & 0 & 0 & \dots \\ 0 & R_{1,2}(g) & 0 & 0 & \dots \\ 0 & 0 & R_{2,1}(g) & 0 & \dots \\ 0 & 0 & 0 & R_{2,2}(g) & \dots \\ \dots & & & & \end{pmatrix}$$

We are going to denote the element in this basis using 3 indices as : $\{|a, j, x\rangle\}$. That is, we can write

$$\langle a, j, x| R(g) |b, k, y\rangle = \delta_{a,b}\delta_{x,y} \left[R_{a,x}(g)\right]_{jk} \tag{7.123}$$

Here $\left[R_{a,x}(g)\right]_{jk}$ is just the j, k element of the matrix for the representation $R_a(g)$. Here:

- $a = 1, 2, 3, \dots$ denote type of representation, i.e. indicate each of the non-equivalent representations $R_1, R_2, R_3, \dots$. At this point: $R_a(g)$ acts in a subspace $\mathcal{H}_a$.
- The same representation can be used multiple times, as we have seen in the previous example. The x index denotes which of these equivalent representation we consider.
- Finally; $\{|a, j, x\rangle\}$ with $j = 1, 2, 3, \dots$ is used to represent a basis within the x_{th} copy of subspace $\mathcal{H}_a$.

7.12.2 How to construct projectors

The question we address in this section is how to construct projectors onto $|a, j, x\rangle$. To do so, we start from

$$R(g) = \oplus_{a,x} R_{a,x}(g) \tag{7.124}$$

and

$$R_{a,x} = \sum_{lm} \langle a, l, x| R(g) |a, m, x\rangle |l\rangle\langle m| = \sum_{lm} [R_a(g)]_{lm} |l\rangle\langle m| \, . \tag{7.125}$$

so applying the representation to the vector $|a, j, x\rangle$ gives:

$$R(g) |a, j, x\rangle = \sum_k [R(a(g)]_{kj} |a, k, x\rangle \, . \tag{7.126}$$

Now we multiply by $[R_b(g)]^*_{k'j'}$ and sum over the group elements to give:

$$\begin{aligned} \sum_g [R_b(g)]^*_{k'j'} R(g) |a, j, x\rangle &= \sum_k \sum_g [R_b(g)]^*_{k'j'} [R(a(g)]_{kj} |a, k, x\rangle \\ &= \sum_k \sum_g [R_b(g)^\dagger]_{j'k'} [R(a(g)]_{kj} |a, k, x\rangle \, . \end{aligned} \tag{7.127}$$

and now, using the grand orthogonality theorem, one finds

$$\begin{aligned}\sum_g [R_b(g)]^*_{k'j'} R(g) |a,j,x\rangle &= \sum_k \frac{N}{n_a} \delta_{jj'}\delta_{kk'}\delta_{ab} |a,k,x\rangle \\ &= \frac{N}{n_a}\delta_{ab}\delta_{jj'} |a,k',x\rangle \,.\end{aligned} \tag{7.128}$$

Thus, we see that we can define

$$\hat{\Pi}^b_{kj} = \frac{n_a}{N}\sum_g [R_b(g)]^*_{kj} R(g) \tag{7.129}$$

such that we have

$$\hat{\Pi}^b_{kj} |a,j,x\rangle = \frac{n_a}{N}\sum_g [R_b(g)]^*_{kj} R(g) |a,j,x\rangle = \delta_{ab} |a,k,x\rangle \tag{7.130}$$

That is this operator satisfies:

$$\hat{\Pi}^a_{kj} |a,j,x\rangle = |a,k,x\rangle \tag{7.131}$$

$$\hat{\Pi}^a_{kj} |b,j',x\rangle = 0 \quad \text{otherwise} \tag{7.132}$$

so that if we know one vector of the basis, then we can find all the other ones! And Π^a_{kk} can be used to find that first vector.

Now, let us take the trace. We find

$$\hat{P}_a = \sum_j \hat{\Pi}^a_{jj} = \sum_g \frac{n_a}{N}\sum_j [R_b(g)]^*_{jj} R(g) = \frac{n_a}{N}\sum_g \chi^*_a(g) R(g) \tag{7.133}$$

This is a projector on the basis of the representation! In other words we have

$$\hat{P}_a = \sum_{j,x} |a,j,x\rangle\langle a,j,x| = \frac{n_a}{N}\sum_g \chi^*_a(g) R(g)\,. \tag{7.134}$$

In summary

- P_a is a projector in the space generated by one irreducible representation, that is the space of all $|a,j,x\rangle$ for all j and x. That is, on the Hilbert space $\mathcal{H}_a = \oplus_x \mathcal{H}_{a,x}$.
- Π^a_{jj} is a projector on the subspace $|a,j,x\rangle$ for all x, but with a fixed j (that is , one of the dimension of the representation).
- Π^a_{kj} is a generalised projector.

As ever let's quickly convince ourselves that this does actually work by looking at a quick example. Consider the Pauli group $G = \{\pm(i)\sigma_x, \pm(i)\sigma_y, \pm(i)\sigma_z, \pm(i)I\}$. We first note that all Pauli's are traceless and so their contribution vanishes leaving us with only the contribution from the identity terms. Thus we have:

$$\begin{aligned}P_a &= \frac{2}{16}(\mathrm{Tr}(I)^* I + \mathrm{Tr}(-I)^*(-I) + \mathrm{Tr}(iI)^*(iI) + \mathrm{Tr}(-iI)^*(-iI)) \\ &= \frac{4}{16}(I+I+I+I) = I\,,\end{aligned} \tag{7.135}$$

as expected. (Note the similarities between this and the group averaging results in Section 7.10).

7.13 Ammonia Molecule Example

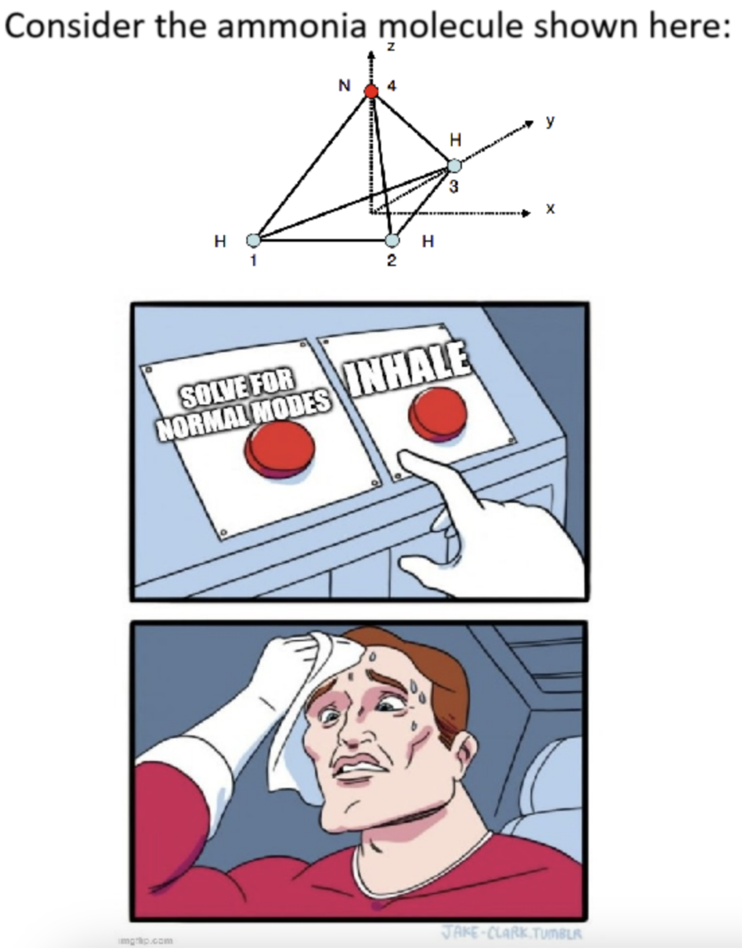


Figure 7.20: Credit: Stefan Visnjic

Let us end by tying everything together with the example of the vibrations modes of the ammonia molecule (NH_3). This will be a classical treatment; however, the lessons carry over to quantum problems. For a more detailed introduction to the symmetry properties of the ammonia molecule see Chapter 1 of Vincenzo Savona's notes. You will also have the pleasure of working through this example in all its gory details in the problem sheet this week. In fact, if you want to take a stab at that problem sheet without any hints, stop reading now and have a go at it first. However, there's quite a bit to put together so I thought this week I'd use the notes to talk you through it.

The ammonia molecule consists of three hydrogen atoms arranged in a triangle and one nitrogen atom located on the vertical axis passing through the center of the triangle (see Figure 7.21). In molecular physics, it is known that for small displacements from the equilibrium positions, the restoring forces on the four atoms are proportional to the displacements. The molecule behaves as a system of coupled harmonic oscillators with 12 degrees of freedom (three spatial coordinates for each atom). Let's denote $\mathbf{R}_1$, $\mathbf{R}_2$, $\mathbf{R}_3$, and $\mathbf{R}_4$ as the coordinates of the three hydrogen atoms and the nitrogen atom. If the equilibrium positions of the four atoms are $\mathbf{R}_j^{(0)}$, where $j = 1, \ldots, 4$, then the displacement vectors are given by $\mathbf{u}_j = \mathbf{R}_j - \mathbf{R}_j^{(0)}$. Let m_H and m_N be the masses of the hydrogen and nitrogen atoms, respectively.

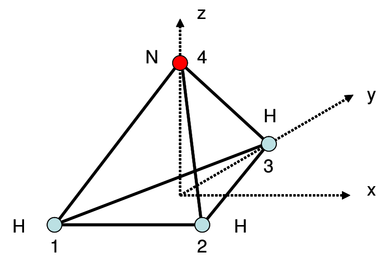


Figure 7.21: Scheme of the NH_3 molecule. In the figure, you can also see the numbering of the four atoms and the choice of the reference frame.

The symmetries of ammonia correspond to the symmetry group of a triangle in 2D. That is, we spot immediately that the relevant symmetry group here is our favourite C3v with group elements: $e, c_+, c_-, \sigma, \sigma', \sigma''$ (i.e., identity, rotations by $\pm 2\pi/3$ and reflections in each of the axis of the triangle). So what is the representation of C3v on the 12 dimensional space spanned by $\boldsymbol{u} := (\mathbf{u}_1, \mathbf{u}_2, \mathbf{u}_3, \mathbf{u}_4)$ corresponding to the spacial displacements of the atoms that ammonia is made up of?

Well the representation of the identity is easy that's just:

$$R(e) = \mathbb{1}_{12\times 12} = \begin{pmatrix} \mathbb{1} & 0 & 0 & 0 \\ 0 & \mathbb{1} & 0 & 0 \\ 0 & 0 & \mathbb{1} & 0 \\ 0 & 0 & 0 & \mathbb{1} \end{pmatrix} \tag{7.136}$$

The c_+ rotation by $2\pi/3$ cyclically rotates molecules 1,2, and 3 (i.e., sends molecule 1 to 3, 2 to 1 and 3 to 2) and corresponds to a $2\pi/3$ rotation about the z axis in the x, y plane. The rotation c_- is just the converse of this. Therefore we have:

$$\begin{aligned} R(c_+) &= \begin{pmatrix} 0 & 0 & S & 0 \\ S & 0 & 0 & 0 \\ 0 & S & 0 & 0 \\ 0 & 0 & 0 & S \end{pmatrix} \qquad \text{with} \quad S = \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix} \\ R(c_-) &= \begin{pmatrix} 0 & S^{-1} & 0 & 0 \\ 0 & 0 & S^{-1} & 0 \\ S^{-1} & 0 & 0 & 0 \\ 0 & 0 & 0 & S^{-1} \end{pmatrix} \quad \text{with} \quad S^{-1} = \begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} & 0 \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix} \end{aligned} \tag{7.137}$$

The σ reflection around the y axis is also easy to spot. This just switches the positions of molecules 1 and 2 and sends $-x$ to x (and vice versa) (see Fig. 7.21) and leaves all other coordinates invariant. Similar analysis can be applied to the σ_2 and σ_3 reflections. Thus we have:

$$R(\sigma) = \begin{pmatrix} 0 & M_1 & 0 & 0 \\ M_1 & 0 & 0 & 0 \\ 0 & 0 & M_1 & 0 \\ 0 & 0 & 0 & M_1 \end{pmatrix} \text{ with } M_1 = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$R(\sigma') = \begin{pmatrix} M_2 & 0 & 0 & 0 \\ 0 & 0 & M_2 & 0 \\ 0 & M_2 & 0 & 0 \\ 0 & 0 & 0 & M_2 \end{pmatrix} \text{ with } M_2 = \begin{pmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} & 0 \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{7.138}$$

$$R(\sigma'') = \begin{pmatrix} 0 & 0 & M_3 & 0 \\ 0 & M_3 & 0 & 0 \\ M_3 & 0 & 0 & 0 \\ 0 & 0 & 0 & M_3 \end{pmatrix} \text{ with } M_3 = \begin{pmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Ok so now we have a representation on the 12d space spanned by the coordinates of the displacements of the ammonia molecule. We expect that this 12d representation is reducible. Indeed we know this as we've already seen that there are 3 irreps of C3v in Section 7.11.1, 2 1D irreps and 1 2D irrep. To save you flicking back I'll just copy them down to here:

The trivial 1D irrep:

$$R_1(e) = 1, R_1(c_+) = 1, R_1(c_-) = 1, R_1(\sigma) = 1, R_1(\sigma') = 1, R_1(\sigma'') = 1 \tag{7.139}$$

The 1D sign irrep:

$$R_2(e) = 1, R_2(c_+) = 1, R_2(c_-) = 1, R_2(\sigma) = -1, R_2(\sigma') = -1, R_2(\sigma'') = -1 \tag{7.140}$$

The 2D irrep:

$$\begin{aligned} R_3(e) &= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \\ R_3(c_+) &= \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}, R_3(c_-) = \begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix} \\ R_3(\sigma) &= \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}, R_3(\sigma') = \begin{pmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}, R_3(\sigma'') = \begin{pmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix} \end{aligned} \tag{7.141}$$

The corresponding C3v character table is shown in Table 7.13.

	e	$2c_+$	$3\sigma_v$
R_1	1	1	1
R_2	1	1	-1
R_3	2	-1	0
R	12	0	2

Table 7.2: Character table for point group C3v.

So how do we write our 12d rep in terms of these irreps? Well we can use Theorem 7.11.3 to compute the number of times each of these irreps appears in our rep. That is, we can use

$$b_a = \frac{1}{N} \sum_{\mu} n_\mu \chi_a^*(C_\mu) \chi_R(C_\mu) \tag{7.142}$$

where b_a is the degeneracy factor of representation a, n_μ is the number of group elements in conjugacy class μ and N is the order of the group. Thus we have

$$\begin{aligned} b_1 &= \frac{1}{6}(1\times 1\times 12 + 2\times 1\times 0 + 3\times 1\times 2) = 3 \\ b_2 &= \frac{1}{6}(1\times 1\times 12 + 2\times 1\times 0 - 3\times 1\times 2) = 1 \\ b_3 &= \frac{1}{6}(1\times 2\times 12 - 2\times 1\times 0 + 3\times 0\times 2) = 4 \end{aligned}$$

And thus, we can express R in terms of the irreducible representations of C_{3v} as follows:

$$R = 3R_1 \oplus R_2 \oplus 4R_3. \tag{7.143}$$

We now know how to compose R into irreps. But we do not yet know the basis to do so. That is, we need to look for a basis where 3×1 vectors are invariant under R_1, where 1×1 vectors are invariant under R_2, and 4×2 vectors are invariant under R_3 [33]. To achieve this, it suffices to choose an arbitrary basis (we choose for simplicity $\boldsymbol{v}_i = \hat{\boldsymbol{e}}_i$ where $\hat{\boldsymbol{e}}_i$ is a normalized vector with the i-th entry being the only non-zero entry) and apply various projectors.

Recall from Eq. (7.129) that a projector onto a basis state of an irrep takes the form:

$$\hat{\Pi}^b_{kj} = \frac{n_b}{N}\sum_g [R_b(g)]^*_{kj} R(g) \tag{7.144}$$

where n_b is the dimension of the representation b and N is the order of the group. That is, we have and we have

$$\hat{\Pi}^a_{kj}\,|a,j,x\rangle = |a,k,x\rangle \tag{7.145}$$

$$\hat{\Pi}^a_{kj}\,|b,j',x\rangle = 0 \quad \text{otherwise} \tag{7.146}$$

where $|a,k,x\rangle$ is a basis for the reduced representation. So if we apply Π^b_{kj} on an arbitrary state and get a non-zero vector, we are left with a (non-normalised) basis state. If we get a set of these we can create an orthonormal basis via the gram-schmidt procedure.

Let us start by constructing the projector corresponding to R_1:

$$\hat{\Pi}^1_{11} = \frac{1}{6}\sum_g [R_1(g)]^*_{11} R(g) = \frac{1}{6}\left(R(e) + R(c_+) + R(c_1) + R(\sigma) + R(\sigma') + R(\sigma'')\right). \tag{7.147}$$

Thus we have:

$$\hat{\Pi}^1_{11} = \frac{1}{6}\begin{pmatrix} \mathbb{1}+M_2 & S^{-1}+M_1 & S+M_3 & 0 \\ S+M_1 & \mathbb{1}+M_3 & S^{-1}+M_2 & 0 \\ S^{-1}+M_3 & S+M_2 & \mathbb{1}+M_1 & 0 \\ 0 & 0 & 0 & S^{(1)} \end{pmatrix} \tag{7.148}$$

where we have defined $S^{(1)} = \mathbb{1} + M_1 + M_2 + M_3 + S + S^{-1}$. Similarly for R_2 we have

$$\hat{\Pi}^2_{11} = \frac{1}{6}\sum_g [R_2(g)]^*_{11} R(g) = \frac{1}{6}\left(R(e) + R(c_+) + R(c_1) - R(\sigma) - R(\sigma') - R(\sigma'')\right). \tag{7.149}$$

[33]By comparison, remember the 2 fold tensor representation of SU(2) decomposed into a direct sum of irreps of irreps on SU(3) and SU(1) *in the Bell basis.* We currently know that $R = 3R_1 \oplus R_2 \oplus 4R_3$ in some basis but we do not know which yet. In our warm up example the three Bell states $\{|\psi_+\rangle, |\phi_+\rangle, |\phi_-\rangle\}$ and

so we have the same as above but get a minus sign in front of each of the M_i terms. That is,

$$\hat{\Pi}^2_{11} = \frac{1}{6}\begin{pmatrix} \mathbb{1}+M_2 & S^{-1}-M_1 & S-M_3 & 0 \\ S-M_1 & \mathbb{1}-M_3 & S^{-1}-M_2 & 0 \\ S^{-1}-M_3 & S-M_2 & \mathbb{1}-M_1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \tag{7.150}$$

where we note that $\mathbb{1}-M_1-M_2-M_3+S+S^{-1}=0$. I'll leave it up to you to compute $\hat{\Pi}^3_{11}$ yourself.

We can now use the projectors to find a basis for each of the irreps. Let us start with R_1. We can find the first 3 basis vectors by evaluating $\boldsymbol{u} \equiv \hat{\Pi}^1_{11}\boldsymbol{v}$ and to give a set of 3 linearly independent vectors $\boldsymbol{u}$ in this basis. One possible choice (not necessarily unique, also dependent on the basis $\boldsymbol{v}_i$) is to select: $\hat{\Pi}^1_{11}\boldsymbol{v}_1$, $\hat{\Pi}^1_{11}\boldsymbol{v}_3$, and $\hat{\Pi}^1_{11}\boldsymbol{v}_{12}$. Then each of these vectors needs to be orthonormalized using, for example, a Gram-Schmidt algorithm. We'll use $\hat{\boldsymbol{u}}$ to denote the vector of the constructed basis after they have been orthonormalized. It's an iterative procedure, before adding a vector to the basis, it needs to be orthonormalized with respect to those already in the basis.

Let's see what this looks like for R_1. We start by evaluating

$$\begin{aligned} \boldsymbol{u}_{1,1} = \hat{\Pi}^1_{11}\boldsymbol{v}_1 &= \frac{1}{6}\begin{pmatrix} \mathbb{1}+M_2 & S^{-1}+M_1 & S+M_3 & 0 \\ S+M_1 & \mathbb{1}+M_3 & S^{-1}+M_2 & 0 \\ S^{-1}+M_3 & S+M_2 & \mathbb{1}+M_1 & 0 \\ 0 & 0 & 0 & S^{(1)} \end{pmatrix}\boldsymbol{v}_1 \\ &= \left(\frac{1}{4},\frac{\sqrt{3}}{12},0,-\frac{1}{4},\frac{\sqrt{3}}{12},0,0,-\frac{\sqrt{3}}{6},0,0,0,0\right) \end{aligned} \tag{7.151}$$

which if we normalise gives

$$\hat{\boldsymbol{u}}_{1,1} = \left(\frac{1}{2},\frac{1}{2\sqrt{3}},0,-\frac{1}{2},\frac{1}{2\sqrt{3}},0,0,-\frac{1}{\sqrt{3}},0,0,0,0\right). \tag{7.152}$$

Let's do another one

$$\boldsymbol{u}_{1,3} \equiv \hat{\Pi}^1_{11}\boldsymbol{v}_{12} = (0,0,0,0,0,0,0,0,0,0,0,1) = \hat{\boldsymbol{u}}_{1,3} \tag{7.153}$$

which conveniently is already normalised and orthogonal to $\hat{\boldsymbol{u}}_{1,1}$. You can similarly generate a third one as

$$\boldsymbol{u}_{1,2} \equiv \hat{\Pi}^1_{11}\boldsymbol{v}_3 \qquad \rightarrow \qquad \hat{\boldsymbol{u}}_{1,2} = \left(0,0,\frac{1}{\sqrt{3}},0,0,\frac{1}{\sqrt{3}},0,0,\frac{1}{\sqrt{3}},0,0,0\right) \tag{7.154}$$

where in this case you need to explicitly apply Gram Schmidt to ensure $\hat{\boldsymbol{u}}_{1,2}$ is normalised and orthogonal to $\hat{\boldsymbol{u}}_{1,1}$ and $\hat{\boldsymbol{u}}_{1,3}$. I've given you the answer above but please do work through and check you get that yourself.

The basis for R_2 is simple as its only 1D. For example, we can just do $\hat{\Pi}^2_{11}\boldsymbol{v}_1$ to get

$$\boldsymbol{u}_{2,1} \equiv \hat{\Pi}^2_{11}\boldsymbol{v}_1 \qquad \rightarrow \qquad \hat{\boldsymbol{u}}_{2,1} = \left(\frac{1}{2\sqrt{3}},-\frac{1}{2},0,\frac{1}{2\sqrt{3}},\frac{1}{2},0,-\frac{1}{\sqrt{3}},0,0,0,0,0\right). \tag{7.155}$$

Finally we come to the basis for R_3. This is more subtle. For R_3, we need to find four pairs of invariant vectors that live in the same invariant subspace. We can do this by creating the first vector using the same procedure as above, i.e. as $\boldsymbol{u} \equiv \Pi^{(3)}_{11}\boldsymbol{v}$ for some $\boldsymbol{v}$. On normalizing we'll have $\hat{\boldsymbol{u}} = |3,1,x\rangle$. Then to find another vector in the same invariant subspace we can take $\boldsymbol{u}' \equiv \Pi_{21}^{(3)}\hat{\boldsymbol{u}}$ such that we have

$$\hat{\Pi}_{21}^{3}\,|3,1,x\rangle \quad = \quad |3,2,x\rangle\,. \tag{7.156}$$

This way we can be sure that $\hat{\boldsymbol{u}}$ and $\hat{\boldsymbol{u}}'$ leave the same invariant subspace. It's a little long to do but works. I'll leave the fun* of doing so to you.

Putting it all together, we end up with a set of ortho-normal vectors. We can then use these to construct the unitary that transforms into the basis in which R decomposes into irreps:

$$\boldsymbol{U} = (\hat{\boldsymbol{u}}_{1,1}, \hat{\boldsymbol{u}}_{1,2}, \hat{\boldsymbol{u}}_{1,3}, \hat{\boldsymbol{u}}_{2,1}, \hat{\boldsymbol{u}}_{3,1}, \hat{\boldsymbol{u}}_{3,2}, \hat{\boldsymbol{u}}_{3,4}, \hat{\boldsymbol{u}}_{3,3}, \hat{\boldsymbol{u}}'_{3,1}, \hat{\boldsymbol{u}}'_{3,2}, \hat{\boldsymbol{u}}'_{3,4}, \hat{\boldsymbol{u}}'_{3,3}) \tag{7.157}$$

Why is this good to know? Well from Schur's lemmas we know that we can use the irrep structure to block diagonalize any operator that commutes with all representations of elements of the group. Thus we see immediately that we can block diagonalize any 12d operator that commutes with $R(g)$ for all g.

Let's look at an example of this. To realistically describe the harmonic modes of the ammonia, a precise parametrization of the elastic constants would be necessary. In general, we cannot express the harmonic force on an atom as the sum of harmonic forces exerted by the other atoms because the harmonic constant for the force between two atoms will be influenced by the presence of the other atoms. However, in the context of this exercise, we can introduce a highly simplified model without fear, which allows us to familiarize ourselves with the symmetry properties. We will assume that the system is simply characterized by two harmonic constants: k_{HH} for the restoring force between two hydrogen atoms and k_{NH} for the force between a hydrogen atom and the nitrogen atom. We have made a strong approximation by assuming that the harmonic force between two atoms is isotropic.

Once the masses and elastic constants are given, we can write the potential energy as follows:

$$\begin{aligned} V(\mathbf{u}_1,\mathbf{u}_2,\mathbf{u}_3,\mathbf{u}_4) \quad &= \quad \frac{1}{2}k_{HH}\left[(\mathbf{u}_1-\mathbf{u}_2)^2+(\mathbf{u}_1-\mathbf{u}_3)^2+(\mathbf{u}_2-\mathbf{u}_3)^2\right] \\ &+ \quad \frac{1}{2}k_{NH}\left[(\mathbf{u}_1-\mathbf{u}_4)^2+(\mathbf{u}_2-\mathbf{u}_4)^2+(\mathbf{u}_3-\mathbf{u}_4)^2\right]. \end{aligned} \tag{7.158}$$

The force acting on a given particle is obtained from the gradient of this potential with respect to the corresponding displacement variable:

$$\mathbf{F}_j = m_j\frac{\partial^2\mathbf{u}_j}{\partial t^2} = -\frac{\partial V}{\partial \mathbf{u}_j}, \tag{7.159}$$

which allows us to write the equations of motion for the system:

$$\begin{aligned} m_H\frac{\partial^2\mathbf{u}_1}{\partial t^2} \quad &= \quad -k_{HH}(\mathbf{u}_1-\mathbf{u}_2)-k_{HH}(\mathbf{u}_1-\mathbf{u}_3)-k_{NH}(\mathbf{u}_1-\mathbf{u}_4)\,, \\ m_H\frac{\partial^2\mathbf{u}_2}{\partial t^2} \quad &= \quad -k_{HH}(\mathbf{u}_2-\mathbf{u}_1)-k_{HH}(\mathbf{u}_2-\mathbf{u}_3)-k_{NH}(\mathbf{u}_2-\mathbf{u}_4)\,, \\ m_H\frac{\partial^2\mathbf{u}_3}{\partial t^2} \quad &= \quad -k_{HH}(\mathbf{u}_3-\mathbf{u}_1)-k_{HH}(\mathbf{u}_3-\mathbf{u}_2)-k_{NH}(\mathbf{u}_3-\mathbf{u}_4)\,, \\ m_N\frac{\partial^2\mathbf{u}_4}{\partial t^2} \quad &= \quad -k_{NH}(\mathbf{u}_4-\mathbf{u}_1)-k_{NH}(\mathbf{u}_4-\mathbf{u}_2)-k_{NH}(\mathbf{u}_4-\mathbf{u}_3)\,. \end{aligned} \tag{7.160}$$

In this simplified notation, it is implied that the variables $\mathbf{u}_j(t)$ depend on time. Such a system of coupled oscillators is characterized by "normal modes." A normal mode is a specific solution to the equations (7.160) where the 12 degrees of freedom depend on time according to the same harmonic law:

$$\mathbf{u}_j(t) = \mathbf{u}_j^{(0)} \sin(\omega t)\,. \tag{7.161}$$

Here, $\mathbf{u}_j^{(0)}$ is a constant vector. By substituting the solution (7.161) into the set of equations (7.160), we obtain:

$$\begin{aligned}
\omega^2 \mathbf{u}_1^{(0)} &= \frac{1}{m_H}\left[k_{HH}(\mathbf{u}_1^{(0)} - \mathbf{u}_2^{(0)}) + k_{HH}(\mathbf{u}_1^{(0)} - \mathbf{u}_3^{(0)}) + k_{NH}(\mathbf{u}_1^{(0)} - \mathbf{u}_4^{(0)})\right],\\
\omega^2 \mathbf{u}_2^{(0)} &= \frac{1}{m_H}\left[k_{HH}(\mathbf{u}_2^{(0)} - \mathbf{u}_1^{(0)}) + k_{HH}(\mathbf{u}_2^{(0)} - \mathbf{u}_3^{(0)}) + k_{NH}(\mathbf{u}_2^{(0)} - \mathbf{u}_4^{(0)})\right],\\
\omega^2 \mathbf{u}_3^{(0)} &= \frac{1}{m_H}\left[k_{HH}(\mathbf{u}_3^{(0)} - \mathbf{u}_1^{(0)}) + k_{HH}(\mathbf{u}_3^{(0)} - \mathbf{u}_2^{(0)}) + k_{NH}(\mathbf{u}_3^{(0)} - \mathbf{u}_4^{(0)})\right],\\
\omega^2 \mathbf{u}_4^{(0)} &= \frac{1}{m_N}\left[k_{NH}(\mathbf{u}_4^{(0)} - \mathbf{u}_1^{(0)}) + k_{NH}(\mathbf{u}_4^{(0)} - \mathbf{u}_2^{(0)}) + k_{NH}(\mathbf{u}_4^{(0)} - \mathbf{u}_3^{(0)})\right].
\end{aligned} \tag{7.162}$$

Subsequently, to simplify the notation, we will represent $\mathbf{u}_j^{(0)}$ as simply $\mathbf{u}_j$. We can define the vector in the 12-dimensional space as:

$$\mathbf{u} = (\mathbf{u}_1;\, \mathbf{u}_2;\, \mathbf{u}_3;\, \mathbf{u}_4)\,. \tag{7.163}$$

The system of equations (7.162) can be expressed in the compact form:

$$A\mathbf{u} = \omega^2 \mathbf{u}\,, \tag{7.164}$$

Here, A is the dynamic matrix of the system, obtained straightforwardly from the form (7.162) of the equation of motion and takes the form:

$$A = \begin{pmatrix} A_{DH} & A_{HH} & A_{HH} & A_{HN}\\ A_{HH} & A_{DH} & A_{HH} & A_{HN}\\ A_{HH} & A_{HH} & A_{DH} & A_{HN}\\ -A_{DN} & -A_{DN} & -A_{DN} & 3A_{DN} \end{pmatrix} \tag{7.165}$$

where we have defined $A_{DH} = a_{DH}\mathbf{1}$, $A_{HH} = a_{HH}\mathbf{1}$, $A_{HN} = a_{HN}\mathbf{1}$ $A_{DN} = a_{DN}\mathbf{1}$ are 3×3 matrices multiples of the identity and $a_{DH} = (2k_{HH} + k_{HN})/m_H$, $a_{HH} = -k_{HH}/m_H$, $a_{HN} = -k_{HN}/m_H$, $a_{DN} = k_{HN}/m_N$.

Exercise: Show this!

To find the normal modes of the molecule we need to solve the eigenvalue problem in Eq. (7.164). That is, we want to diagonalize A. We can use our new found knowledge of the irreps of R to do this. That is, the matrix $\tilde{A} = U^\dagger A U$ (where U is the basis change we worked so hard to find earlier in Eq. (7.157)) is block-diagonal:

$$\tilde{A} = \begin{pmatrix} \tilde{A}_{1\times1} & & & & & & \\ & \tilde{A}_{2\times2} & & & & & \\ & & \tilde{A}_{1\times1} & & & & \\ & & & \tilde{A}_{3\times3} & & & \\ & & & & \tilde{A}_{1\times1} & & \\ & & & & & \tilde{A}_{3\times3} & \\ & & & & & & \tilde{A}_{1\times1} \end{pmatrix} \tag{7.166}$$

with :

$$\tilde{A}_{1\times 1} = \frac{3k_{\mathrm{HH}} + k_{\mathrm{HN}}}{m_{\mathrm{H}}} \tag{7.167}$$

$$\tilde{A}_{2\times 2} = \begin{pmatrix} \frac{k_{\mathrm{HN}}}{m_{\mathrm{H}}} & -\frac{\sqrt{3}k_{\mathrm{HN}}}{m_{\mathrm{H}}} \\ -\frac{\sqrt{3}k_{\mathrm{HN}}}{m_{\mathrm{N}}} & \frac{3k_{\mathrm{HN}}}{m_{\mathrm{N}}} \end{pmatrix} \tag{7.168}$$

$$\tilde{A}_{3\times 3} = \begin{pmatrix} \frac{3k_{\mathrm{HH}}+5k_{\mathrm{HN}}}{5m_{\mathrm{H}}} & \frac{6k_{\mathrm{HH}}}{5m_{\mathrm{H}}} & -\frac{2\sqrt{\frac{3}{5}}k_{\mathrm{HN}}}{m_{\mathrm{H}}} \\ \frac{6k_{\mathrm{HH}}}{5m_{\mathrm{H}}} & \frac{12k_{\mathrm{HH}}+5k_{\mathrm{HN}}}{5m_{\mathrm{H}}} & \frac{\sqrt{\frac{3}{5}}k_{\mathrm{HN}}}{m_{\mathrm{H}}} \\ -\frac{2\sqrt{\frac{3}{5}}k_{\mathrm{HN}}}{m_{\mathrm{N}}} & \frac{\sqrt{\frac{3}{5}}k_{\mathrm{HN}}}{m_{\mathrm{N}}} & \frac{3k_{\mathrm{HN}}}{m_{\mathrm{N}}} \end{pmatrix} \tag{7.169}$$

The rows in the matrix $\tilde{A}$ separate the different invariant subspaces R_i. **Exercise: Show this!**

Thus we see that the use of group theory has reduced a problem consisting of diagonalizing a 12×12 matrix to a problem requiring the diagonalization of a 2×2 matrix and a 3×3 matrix, which is much simpler!

Now we can use some physical arguments to intuitively understand what will happen if we fully solve the problem. For example, we noticed that the system is invariant under translation, so a translation along z should not cost any energy. To see this, let's look in the subspace related to Γ_1 and search for a null mode. Clearly, $\tilde{A}_{1\times 1}$ is not zero, so $\tilde{A}_{2\times 2}$ must have a zero eigenvalue. Moreover, by cleverly combining $\hat{\boldsymbol{u}}_{1,2}$ and $\hat{\boldsymbol{u}}_{1,3}$, we can generate the vector $(0,0,1/2,0,0,1/2,0,0,1/2,0,0,1/2)$, which is effectively a translation of each atom along z. To find the other two null modes related to translations along x and y, we need to look in Γ_3. We will find that $\tilde{A}_{3\times 3}$ must also have a zero eigenvalue.

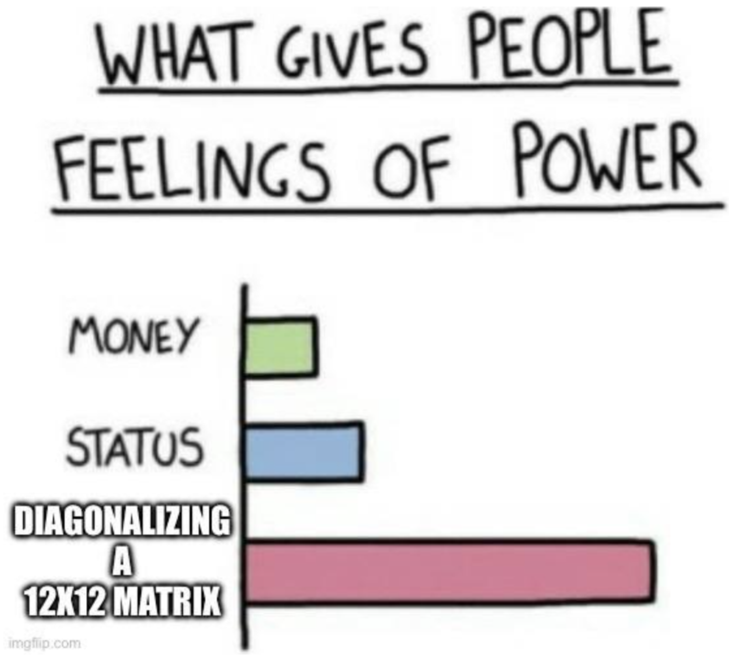


Figure 7.22: Credit: L'heure est grave

Appendices

7.14 Properties of functions

Consider two sets, X and Y. A *function* (or *map*) f from X to Y is defined such that, for each element x belonging to X (denoted as $x \in X$), there exists a unique element y in Y associated with x. We represent this element as $y = f(x)$ and call it the image of x under the function f. We write it as:

$$f : \; X \to Y \quad , \quad x \mapsto y = f(x) \, . \tag{7.170}$$

The set X is called the *domain* of f, and Y is its *image*. The set of elements in Y, which are images under f of elements in X, is called the image of X under f and is denoted as $f(X)$. In general, $f(X)$ is a subset of Y (we write $f(X) \subset Y$) and is not necessarily identical to Y.

The function f is *injective* if:

$$f(x) = f(x') \;\; \Rightarrow \;\; x = x' \, . \tag{7.171}$$

For an injective function, two elements of X cannot have the same image in Y. A function is *surjective* if $f(X) = Y$. For a surjective function, every element of Y is the image of at least one element of X. A function that is both injective and surjective is called *bijective*.

Let f be a function from X to Y and g be a function from Y to Z. The *composition* or *product* of these two functions $h : X \to Z$ is defined as:

$$h(x) = g\left(f(x)\right) \, . \tag{7.172}$$

The function h acts from X to Z and is denoted as:

$$h = g * f \tag{7.173}$$

or simply gf when there is no possibility of confusion with other operations. It should be noted that $f * g$ is not necessarily well-defined, and when it exists, it is not necessarily equal to $g * f$. For example, consider real-valued functions $f(x) = x^2$ and $g(y) = \mathrm{e}^y$. We have:

$$(g * f)(x) = g\left(x^2\right) = \mathrm{e}^{x^2} \tag{7.174}$$

and

$$(f * g)(x) = f\left(\mathrm{e}^x\right) = \mathrm{e}^{2x} \, . \tag{7.175}$$

The composition of functions is associative, meaning that if u, v, and w are functions from X to Y, Y to Z, and Z to W, respectively, then:

$$(w * (v * u))(x) = ((w * v) * u)(x) \, . \tag{7.176}$$

For each $x \in X$, both sides of this equation correspond to the element:

$$w(v(u(x))) \tag{7.177}$$

in W. Therefore, we can write:

$$(w * (v * u))(x) = ((w * v) * u)(x) = w * v * u \, . \tag{7.178}$$

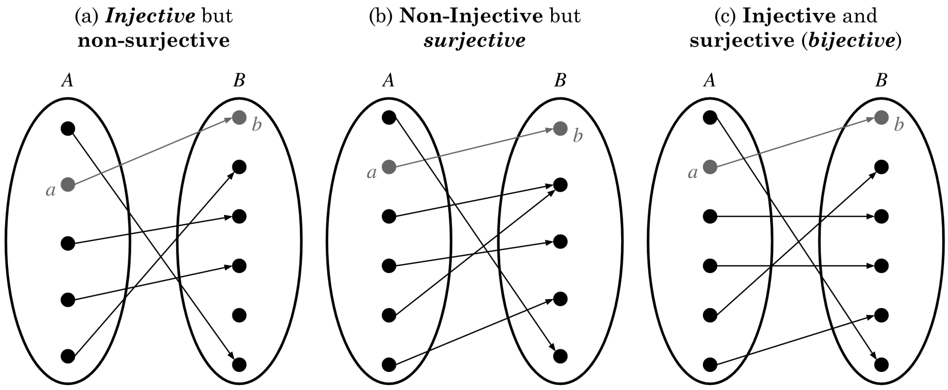


Figure 7.23: Diagram of injective, surjective and bijective functions: (Wiki page on functions).)

If $f : X \to Y$ is a bijective application, then for each element y in Y, there is a unique element x in X such that $f(x) = y$, and, naturally, each element x has an image in Y. Therefore, we can define a bijective application $Y \to X$, $y \mapsto x$ such that $y = f(x)$. This application is called the *inverse* of f and is denoted by f^{-1}.

Often, we consider applications from a set X to itself. An example is given by real (complex) functions of a real (complex) variable. We define the identity application as:

$$e: \ X \to X \quad , \quad x \mapsto e(x) = x \, . \tag{7.179}$$

This application is clearly bijective. If $f : X \to Y$ is a bijective application, f^{-1} exists, and we have:

$$(f^{-1} * f)(x) = x \tag{7.180}$$

for each x. Therefore, we write:

$$f^{-1} * f = e_X \tag{7.181}$$

where we denote the identity application of X by e_X. Note that we also have:

$$f * f^{-1} = e_Y \tag{7.182}$$

Theorem. Let X and Y be two sets containing the same finite number n of elements[34]. The following three statements are equivalent:

(i) $f : X \to Y$ is surjective,

(ii) $f : X \to Y$ is injective,

(iii) $f : X \to Y$ is bijective.

Proof:

(i) $\Rightarrow f(X) = Y$. Thus, $f(X)$ is composed of n elements, which implies (ii).

(ii) $\Rightarrow f(X)$ is composed of n elements. It follows that $f(X) = Y$, which can be reduced to property (i).

Since (i) and (ii) are each a consequence of the other, (iii) is also true, and the theorem is thus proved.

[34]Note that this theorem is not valid for two sets with different numbers of elements.

7.14.1 Proof of Lagrange Theorem, Right and Left cosets

Let G be a group and H one of its proper subgroups. We can define an equivalence relation —different from the last one— between the elements of G as follows: if $x, y \in G$ and $x^{-1}y \in H$ then x and y are equivalent and we write $x \sim y$.

This is indeed an equivalence relation:

- $a^{-1}a = e\ \forall a \in G$, and $e \in H$, so that $a \sim a$.
- if $a \sim b$ then $a^{-1}b \in H$. The inverse of $a^{-1}b$ is $b^{-1}a$ and since H is a group, $b^{-1}a \in H$, so that $b \sim a$.
- if $a \sim b$ and $b \sim c$, then $a^{-1}b$ and $b^{-1}c$ are both in H, thus so is the their product $a^{-1}bb^{-1}c = a^{-1}c$.

This equivalence relation therefore makes it possible to divide the elements of G into disjoint classes. If $x^{-1}y \in H$, then y is equal to an element of H multiplied on the left by x. We indicate the set thus constructed by the symbol

$$C_x = xH \tag{7.183}$$

which the call the *left co-set associated to x*.

The map $H \to xH$ is one-to-one (bijective). Indeed, each element $z \in xH$ is the image of $x^{-1}z \in H$ so that the map is surjective. But the map is also injective since for $y, y' \in H$, we have $xy = xy' \Rightarrow y = y'$.

We could also define a second equivalence relation $x \sim y$ if $yx^{-1} \in H$ and which this case, we can define the concept of right co-set Hx in the same way as before.

These concepts are very useful, and allows in particular to prove Lagrange Theorem:

Demo. Consider the co-sets on the left of H. They are all disjoint or identical (since they are equivalence classes). If there are n distinct left co-sets, their union is G. So, if we denote by g and h the orders of G and H respectively, then $g = nh$ and the theorem is proved. ☐

Let us give an example for the following order 4 group

$$G = \begin{array}{c|cccc} * & e & a & b & c \\ \hline e & e & a & b & c \\ a & a & e & c & b \\ b & b & c & e & a \\ c & c & b & a & e \end{array} \tag{7.184}$$

that has the subgroup $H = \{e, a\}$:

$$H = \begin{array}{c|cc} * & e & a \\ \hline e & e & a \\ a & a & e \end{array} \tag{7.185}$$

We can now construct the left co-sets:

$$C_e = eH = \{e, a\} \tag{7.186}$$
$$C_a = aH = \{a, e\} = C_e \tag{7.187}$$
$$C_b = bH = \{b, c\} \tag{7.188}$$
$$C_c = cH = \{c, b\} = C_b \tag{7.189}$$

And we see indeed that we have *two* left co-set of order 2.

7.15 Composition of Conjugacy classes theorem statement and proof

Theorem 7.15.1 ("Composition" of conjugacy classes)**.** *Let G be a group, and C_x and C_y two of its conjugacy classes. Then we have*

$$C_\nu * C_\mu = \sum_\lambda n_{\mu\nu\lambda} C_\lambda \tag{7.190}$$

with $n_{\mu\nu\lambda}$ integer. Here the multiplication $C_\nu * C_\mu$ is defined as the entire set $[xy]$ for all $x \in C_\nu$ and $y \in C_\mu$. Additionally, $n_{\nu\mu\lambda} = n_{\mu\nu\lambda}$ and $n_{1\nu\lambda} = n_{\nu 1\lambda} = \delta_{\nu,\lambda}$.

To prove this, let us first prove a variant of the reordering theorem:

Theorem 7.15.2 (Reordering theorem within conjugacy classes)**.** *Let G be a group, m one of its elements, and C one of the conjugate classes. Then the application $C \to m^{-1}Cm$ is bijective into itself: The ensemble $m^{-1}Cm$ is thus a re-ordering of C.*

Demo. First notice that this is a map into itself since for any $y \in C$, $m^{-1}ym \in C$ (conjugacy class property). Second, the map is surjective. Indeed, for any $y \in C$, it exists $x = mym^{-1} \in G$ such that $y = m^{-1}xm$. By definition, x is thus also in C and therefore for all $y \in C$ there is an antecedent in C. Third, the map $x \to mx$ is injective (it maps distinct elements to distinct elements). For any x, x', we have $m^{-1}xm = m^{-1}x'm$ implies that $mm^{-1}xmm^{-1} = mm^{-1}x'mm^{-1}$ so that $x = x'$. □

We shall soon prove that $n_{\nu\mu\lambda}$ is indeed an integer. But first, let us note indeed that $n_{\nu\mu\lambda} = n_{\mu\nu\lambda}$, because the two sets $C_\nu * C_\mu$ and $C_\mu * C_\nu$ are identical. Indeed

$$C_\nu * C_\mu = [uv] = \left[uv(u^{-1}u)\right] = \left[u(vu^{-1}u)\right] = \left[uvu^{-1}u\right] = \left[(uvu^{-1})u\right] = C_\mu * C_\nu$$

since u represents all the element of C_ν, and since, from the previous theorem, (uvu^{-1}) represent a re-ordering of the all the element of C_μ as v changes. Additionally, we also see that, denoting the class that contains e are C_1, that $C_1 * C_\nu = C_\nu$ so that $n_{1\nu\lambda} = n_{\nu 1\lambda} = \delta_{\nu,\lambda}$.

Let us now prove that $n_{\nu\mu\lambda}$ is an integer. First we prove the following lemma:

Lemme 7.15.3. *A necessary and sufficient condition for a set $[R]$ to be composed uniquely of a set of entire classes of a group G is that*

$$\forall u \in G\,,\; u^{-1}[R]u = [R]$$

Demo. The condition is necessary because, if indeed $[R]$ is composed of entire sets, then in each of these sets S, $u^{-1}[S]u$ is itself the set S by the reordering theorem.
To see that the condition is sufficient, let us proceed by contradiction and write

$$[R] = [R'] + [R'']$$

where $[R']$ is the largest subset of $[R]$ made of entire classes, and the reminder $[R'']$ thus must contain elements that are not an entire class. Since $[R']$ satisfy $u^{-1}[R']u = [R']$ then

$$u^{-1}[R'']u = [R'']\,.$$

e cannot be in $[R'']$ since it is, itself, a class. Let us suppose $[R'']$ is not empty, and $x \in [R'']$. Then it must exists $y \in G$, conjugated to x, which is *not* in $[R'']$. Since y is conjugated to x we have $u^{-1}xu = y$ for some $u \in G$. But then since $u^{-1}[R'']u = [R'']$ for all u, y must be in $[R'']$. We have thus reach a contradiction, and $[R'']$ is empty. □

Now we can proceed. Let H be a finite group of order h and conjugacy classes $C_1 = \{e\}$, $C_2, \ldots, C_\mu, \ldots, C_{N_C}$ its classes. We shall denote by n_μ the number of elements in the class C_μ and by N_C the total number of classes. We have, of course

$$\sum_{\mu=1}^{N_c} n_\mu = h \tag{7.191}$$

Let C_μ and C_ν be two classes of H, and consider the product

$$C_\mu * C_\nu = [uv] \tag{7.192}$$

where u and v are elements of C_μ and C_ν. Then for each $x \in H$, we have

$$x^{-1}C_\mu * C_\nu x = [x^{-1}uvx] = [x^{-1}u(xx^{-1})vx] = [(x^{-1}ux)(x^{-1}vx)] \tag{7.193}$$

Using the theorem of rearrangement, we see that $[(x^{-1}ux)(x^{-1}vx)]$ is just a reordering of $[uv]$ so that

$$x^{-1}C_\mu * C_\nu x = C_\mu * C_\nu \tag{7.194}$$

Applying lemma 7.15.3 then prove theorem 7.15.1.

7.16 Proof of Schur's lemma

Let us prove Schur's lemma. We are going to need the definition of "kernel" and "image" of an operator.

Definition 7.16.1 (Kernel of an operator)**.** The kernel Ker$A$ of an operator $A : V_1 \to V_2$ is the set of vector $\boldsymbol{v}_1 \in V_1$ such that $Av_1 = 0$.

Definition 7.16.2 (Image of an operator)**.** The image ImA of an operator $A : V_1 \to V_2$ is the set of vector $\boldsymbol{v}_2 \in V_2$ for which $\exists v_1 \in V_1$ such that $v_2 = Av_1$.

Theorem 7.16.3 (Rank-Nullity theorem)**.** *For any operator* $A : V_1 \to V_2$*, define* $\mathrm{Rank}(A) = \dim[\mathrm{Im}(A)]$ *and* $\mathrm{Nullity}(A) = \dim[\mathrm{Ker}(A)]$*, then* $\dim[V_1] = \mathrm{Nullity}(A) + \mathrm{Rank}(A)$.

7.16.1 Proof of lemma 1

Demo. For all $g \in G$ we have:

- $\forall \boldsymbol{v}_1 \in \mathrm{Ker}A$ we have $A(R_1(g)\boldsymbol{v}_1) = R_2(g)A\boldsymbol{v}_1 = 0$. This means that the vector $R_1(g)\boldsymbol{v}_1$ is also in the kernel of A. In other words a vector in $W = \ker A$ stays in W upon transformation by $R_1(g), \forall g$: W is thus a stable sub-space of $R_1(g)$.
- From a similar reasoning, we can deduce that the image $W' = \mathrm{Im}A$ is also a stable subspace for $R_2(g)$. Indeed, this requires implies that if a vector can be written as $\boldsymbol{v}_2 = A\boldsymbol{v}_1$, then $R_2(g)\boldsymbol{v}_2$ can also be written as $A\boldsymbol{v}_1'$. This is the case since $R_2(g)\boldsymbol{v}_2 = R_2(g)A\boldsymbol{v}_1 = AR_1(g)\boldsymbol{v}_1 = A\boldsymbol{v}'$.

We thus conclude that $W = \mathrm{Ker}A$ is a stable subspace $R_1(g)$ and that $W' = A$ is a stable subspace of $R_2(g)$. However, by assumption, both representations are irreducible, so the only subspaces are either 0 or the entire space. We thus have either:

- $\mathrm{Ker}A = 0$, in which case the image is not empty, so that $\mathrm{im}A = V_2$. But this implies that the transformation A is invertible, but then $A^{-1}R_2(g)A = R_1(g)\forall g$, and R_2 and R_1 are equivalent, which contradicts the hypothesis.
- $\mathrm{Ker}A = V_1$, in which case $A = 0$ (and the image is empty:$\mathrm{im}A = 0$).

□

7.16.2 Proof of lemma 2

In this case, we have a map between either the same, or between equivalent representations. Additionally, $V_1 = V_2 = V$, and A is a square matrix. If the representation are equivalent, we can always rotate the space so that they are indeed identical.

Let us consider then that $R_1(g) = R_2(g) = R(g) \forall g$.

Demo. By the fundamental theorem of algebra, it exists an eigenvalue $\lambda \in \mathbb{C}$ such that $\det(A - \lambda I) = 0$. Consider then the equation

$$(A - \lambda I)R(g) = R(g)(A - \lambda I)\,. \tag{7.195}$$

so that if $v \in \mathrm{Ker}(A - \lambda I)$ then $R(g)v$ also in $\mathrm{Ker}(A - \lambda I)$. $W = \mathrm{Ker}(A - \lambda I)$ is thus a stable subspace of transformation by $R(g)\forall g$. Given $R(g)$ is irreducible, either $W = 0$ or $W = V$. W cannot be zero, because at least the eigenvector of A corresponding to λ is in W! Therefore $W = V$.

We this have $\mathrm{Ker}(A - \lambda I) = V$, so that $(A - \lambda I) = 0$ and therefore $A = \lambda I$. □

7.17 Proof of grand orthogonality Lemma

Demo. Consider any matrix X and the matrix M defined as

$$M = \sum_{g\in G} R_1(g^{-1}) X R_2(g) \tag{7.196}$$

Then we have, for any $y \in G$

$$\begin{aligned}
MR_2(y) &= \sum_{g\in G} R_1(g^{-1}) X R_2(g) R_2(y) \\
&= \sum_{g\in G} R_1(y) R_1(y^{-1}) R_1(g^{-1}) X R_2(g) R_2(y) \\
&= R_1(y) \sum_{g\in G} R_1(y^{-1}) R_1(g^{-1}) X R_2(g) R_2(y) \\
&= R_1(y) \sum_{g\in G} R_1(y^{-1} g^{-1}) X R_2(gy) \\
&= R_1(y) \sum_{g\in G} R_1((gy)^{-1}) X R_2(gy) \\
&= R_1(y) \sum_{h\in G} R_1(h^{-1}) X R_2(h) = R_1(y) M
\end{aligned}$$

We can thus use Schur's lemmas on M. Since R_1 and R_2 are not equivalent we have $M = 0$ so that

$$\sum_{g\in G} \sum_{jl} [R_1(g^{-1})]_{kj} X_{jl} [R_2(g)]_{lm} = 0 \tag{7.197}$$

but $R_1(g^{-1})$ is $R_1(g)^\dagger$ so that

$$\begin{aligned}
\sum_{g\in G} \sum_{jl} [R_1(g)]^\dagger_{kj} X_{jl} [R_2(g)]_{lm} &= 0 \\
\sum_{g\in G} \sum_{jl} [R_1(g)]^*_{jk} X_{jl} [R_2(g)]_{lm} &= 0
\end{aligned} \tag{7.198}$$

Using $X_{jl} = 0$ except for one pair jl for which $X_{jl} = 1$ leads to eq.(7.83).

We now turn to eq.(7.85). If we construct the matrix M using the same representation, we get again $MR(x) = R(x)M$ and by the second Schur lemma:

$$\sum_{g\in G} R(g^{-1})XR(g) = c(X)I \tag{7.199}$$

which, in full matrix notation, means

$$\sum_{g\in G}\sum_{jl}[R(g)]^*_{jk}X_{jl}[R(g)]_{lm} = c(X)\delta_{km}$$

We just need to compute the constant. Let us work on the diagonal, when $k = m$, and sum over k so that we have

$$\begin{aligned}
\sum_{g\in G}\sum_{jlk}[R(g^{-1})]_{kj}X_{jl}[R(g)]_{lk} &= n_a c(X)\\
\sum_{g\in G}\sum_{jl}X_{jl}\sum_{k}[R(g^{-1})]_{kj}[R(g)]_{lk} &= n_a c(X)\\
\sum_{g\in G}\sum_{jl}X_{jl}[R(g)R(g^{-1})]_{lj} &= n_a c(X)\\
\sum_{g\in G}\sum_{jl}X_{jl}I_{lj} &= n_a c(X)\\
\sum_{g\in G}\mathrm{Tr}X &= n_a c(X)\\
c(X) &= \frac{N}{n_A}\mathrm{Tr}X
\end{aligned}$$

Using again $X_{jl} = 0$ except for one pair jl for which $X_{jl} = 1$ leads to eq.(7.85). □

7.18 Proof of Burnside Lemma

We can now prove Burnside lemma. Consider the regular representation (which we introduced in the previous chapter) that is obtained using $N \times N$ matrices for a finite group of order N. Then we have a amazing fact: Any irreducible representation D of G appears in the regular representation $dim(D)$ times:

Theorem 7.18.1 (Regular representation decomposition)**.** *Consider the regular representation of a group. Then we have the following decomposition in irrep*

$$R^r(g) = \oplus_{a,x}R_{a,x}(g) = \oplus_a R_a R_a(g) \tag{7.200}$$

where R_a is the dimension of the representation a.

Demo. We simply apply

$$b_a = \frac{1}{N}\sum_{\mu} n_\mu \chi_a^*(C_\mu)\chi^r(C_\mu) \tag{7.201}$$

and using the fact that for the regular representation all characters are zero except for the one corresponding to e, we find

$$b_a = \frac{1}{N}\chi_a^*(C_e) = \frac{R_a}{N}N = R_a \tag{7.202}$$

□

This finally allows to prove Burnside's lemma, by simply counting the dimensions:

Lemme 7.18.2 (Burnside lemma)**.**

$$\sum_{i=1}^{N_r} d_i^2 = N \tag{7.203}$$

7.19 Representations of Lie Groups and Lie Algebras

The following theorems hold on the relationship between representations of Lie groups and Lie algebras [35]:

Theorem 7.19.1 ((Lie group reps induce Lie algebra reps))**.** *Let G be a matrix Lie group with Lie algebra $\mathfrak{g}$. If R is a representation of G on V, then there exists a unique representation r of $\mathfrak{g}$ on V given by*

$$r(J) = \frac{d}{dt}(R(e^{tX}))\bigg|_{t=0}, \text{ for all } X \in \mathfrak{g}. \tag{7.204}$$

We call r the representation of $\mathfrak{g}$ induced by R.

Theorem 7.19.2 ((Lie algebra reps lift to simple Lie group representations))**.** *Let G be a simply connected matrix Lie group, and let r be a representation of the corresponding Lie algebra on V. Then there is a unique representation R of G with the property*

$$R(e^X) = e^{r(X)}, \text{ for all } X \in \mathfrak{g}. \tag{7.205}$$

Theorem 7.19.3 ((Lie algebra reps locally lift to Lie group reps).)**.** *Let G be a matrix Lie group, and let r be a representation of the corresponding Lie algebra on V. Then using Theorem 1, we can always locally define a representation R on G by the mapping*

$$R(g) = e^{r(X)}, \text{ defined for all } g = e^X \text{ nearby } I. \tag{7.206}$$

Here, by "nearby" we mean "wherever the exponential map is a diffeomorphism". Indeed, in this region, all g can be written as $g = e^X$.

[35] These statements are taken from Representation Theory for Geometric Quantum Machine Learning - see there for further discussion.

7.20 Examples of symmetries of quantum models

Here I show a list of examples of quantum models and their symmetries taken from Representation Theory for Geometric Quantum Machine Learning. While these examples are framed in a QML context they are more widely applicable.

Example 11: Discrete symmetries

Bit parity with bit-flip symmetry: Let n be an even number of qubits. Consider a problem of classifying computational basis product states according to their parity. Here, $\rho_i = |\psi_i\rangle\langle\psi_i|$, with $|\psi_i\rangle = |z_{i_1} z_{i_2} \dots z_{i_n}\rangle$, and where $z_{i_k} \in \{0,1\}$ the parity of $|\psi_i\rangle$ is defined as $y_i = f(|\psi_i\rangle) = \sum_{k=1}^n z_{i_k} \mod 2$. Defining the spin-flip operator $P = \bigotimes_{j=1}^n X_j$, where X_j is the Pauli-x operator acting on the j-th qubit. One can readily see that while $P|\psi_i\rangle \neq |\psi_i\rangle$, the parity is invariant under P, i.e. $f(P|\psi_i\rangle) = f(|\psi_i\rangle)$. For a concrete example, $f(P|01\rangle) = 1 = f(|10\rangle)$. In other words, the states are not invariant under the symmetry, but the labels are.

- *States:* Bitstring product states $|\psi_i\rangle = |z_{i_1} z_{i_2} \dots z_{i_n}\rangle \in (\mathbb{C}^2)^{\otimes n}$, where $z_{i_k} \in \{0,1\}$ and n even
- *Labels:* Parity $y_i = f(|\psi_i\rangle) = \sum_{k=1}^n z_{i_k} \mod 2$
- *Group:* $\mathbb{Z}_2 = \{1, p\}$
- *Representation:* $R : G \mapsto GL((\mathbb{C}^2)^{\otimes n})$, where $1 \cdot |\psi_i\rangle = |\psi_i\rangle$, $\sigma \cdot |\psi_i\rangle = P|\psi_i\rangle$

Qubit reflection parity: Consider a problem of classifying states according to their qubit-reflection parity. Defining the qubit-reflection operator $R := R_{1,n} R_{2,n-1} \dots R_{\lfloor n/2 \rfloor, \lfloor n/2 \rfloor+1}$, where $R_{j,j'}$ swaps qubits j and j', and writing $\rho_i = |\psi_i\rangle\langle\psi_i|$, the states will have label $y_i = 0$ ($y_i = 1$) if ρ_i is an eigenstate of R with eigenvalue 1 (-1). Here, one can readily verify that $R\rho_i R^\dagger = \rho_i$.

Qubit permutations: Learning problems with permutation symmetries abound. Examples include learning over sets of elements, modeling relations between pairs (graphs) or multiplets (hypergraphs) of entities, problems defined on grids (such as condensed matter systems), molecular systems, evaluating genuine multipartite entanglement, or working with distributed quantum sensors. Consider for instance a problem where an n-qubit ρ is a graph state encoding the topology of an underlying graph. One can create such state by starting with the state $|+\rangle^{\otimes n}$, and applying a unitary $U^{(a,b)}$ for each edge (a,b) in the graph. Here $U^{(a,b)} = e^{-i\gamma((|0\rangle\langle 0|)^a \otimes \mathbb{1}^b + (|1\rangle\langle 1|)^a \otimes Z^b)}$ is an Ising-type interaction. By conjugating the state with an element of S_n, one obtains a new quantum state whose interaction graph is isomorphic to the original one.

- *States:* Quantum states on qubits, where the qubit labeling index do not matter.
- *Labels:* *(Here, any label will work, since the states themselves are invariant).*
- *Group:* $G = S_n$, the symmetric group on n letters
- *Representation:* $R : G \mapsto GL((\mathbb{C}^2)^{\otimes n})$, where the 2-cycle $(j,j') \cdot |\psi_i\rangle = \mathrm{SWAP}_{j,j'}|\psi_i\rangle$. Note that since any permutation in S_n can be expressed as a product of swaps, this defines our representation on all permutations.

Translation invariance: Let H a Hamiltonian and consider the problem of classifying energies y_i of a set of eigenstates $|\psi_i\rangle$. Suppose $H = \sum_{j=1}^n h_{j,j+1}$, where $h_{j,j+1}$ is a nearest-neighbor interaction and we impose periodic boundary conditions so that $n+1 \equiv 1$. Then H commutes with the translation operator $\tau_g : (\mathbb{C}^2)^{\otimes n} \to (\mathbb{C}^2)^{\otimes n}$, which translates the state $|\psi\rangle$ to the right by g sites (e.g. $\tau_0 = \mathbb{1}$ and $\tau_2|01101\rangle = |01011\rangle$). We can then use Prop. 5 to argue that the energy label y_i is invariant under the group of translations, so $f(|\psi_i\rangle) = f(\tau_g|\psi_i\rangle)$ for all translations τ_g.

- *States:* Eigenstates $|\psi_i\rangle$ of a Hamiltonian H on a ring of n qubits
- *Labels:* Eigenenergies y_i, i.e. $H|\psi_i\rangle = y_i|\psi_i\rangle$
- *Group:* $G = \mathbb{Z}_n$, the cyclic group of order n.
- *Representation:* $\tau : G \mapsto GL((\mathbb{C}^2)^{\otimes n})$, where τ_g translates to the right by g sites

Figure 7.24:

Example 12: Continuous symmetries

Unitary transformations and purity: Consider a problem of classifying pure states from mixed states. The dataset here is composed of states with label $y_i = 0$ ($y_i \neq 0$) if ρ_i is pure (mixed). Since the purity is a spectral property, then the labels in $\mathcal{S}$ are invariant under the action of any unitary. Note that here $f(U\rho_i U^\dagger) = f(\rho_i)$, but in general $U\rho_i U^\dagger \neq \rho_i$.

- *States:* States $\rho_i \in \mathcal{D}(\mathcal{H})$.
- *Labels:* Pure $y_i = 0$ and mixed $y_i \neq 0$.
- *Group:* $G = U(d)$, the unitary group on $\mathcal{H}$.
- *Representation:* $U : G \mapsto U(d)$, where $g \cdot \rho_i = U_g \rho_i U_g^\dagger$.

Orthogonal transformations: Consider a problem of classifying orthogonal (real-valued) states from Haar-random states. The dataset here is composed of states with label $y_i = 0$ ($y_i \neq 0$) if ρ_i is a real-valued state (a Haar random state). Here, the labels $y_i = 0$ are invariant under the action of any orthogonal unitary, as conjugated a real-valued state by a real-valued unitary yields a real-valued state. Note that here $f(U\rho_i U^\dagger) = f(\rho_i)$, but in general $U\rho_i U^\dagger \neq \rho_i$.

- *States:* States $\rho_i \in \mathcal{D}(\mathcal{H})$.
- *Labels:* Orthogonal $y_i = 0$ and mixed $y_i \neq 0$.
- *Group:* $G = O(d)$, the orthogonal group on $\mathcal{H}$
- *Representation:* $U : G \mapsto O(d)$, where $g \cdot \rho_i = U_g \rho_i U_g^\dagger$

Local unitary transformations and the XXX model: Consider the problem of classifying ground states of the Heisenberg XXX model $H = J\sum_{j=1}^n (X_j X_{j+1} + Y_j Y_{j+1} + Z_j Z_{j+1})$. Here, $y_i = 0$ ($y_i = 1$) if ρ_i is a ferromagnetic (antiferromagnetic) ground state of H with $J < 0$ ($J > 0$). Since H commutes with the total magnetization operators $S_x = \sum_{j=1}^n X_j$, $S_y = \sum_{j=1}^n Y_j$, $S_z = \sum_{j=1}^n Z_j$, then the labels are invariant under the action of the same local unitary acting on all qubits. That is, $f((\bigotimes_i^n U)\rho_i(\bigotimes_i^n U^\dagger)) = f(\rho_i)$ for any local unitary U.

- *States:* Ground states of the XXX chain $\rho_i \in \mathcal{D}(\mathcal{H})$
- *Labels:* Ferromagnetic $y_i = 0$ and antiferromagnetic $y_i = 1$
- *Group:* $G = U(2)$
- *Representation:* $U : G \mapsto U(d)$, where $g \cdot \rho_i = (U_g \otimes \cdots \otimes U_g)\rho_i(U_g \otimes \cdots \otimes U_g)^\dagger$

Local unitary transformations and multipartite entanglement: Consider the problem of classifying pure quantum states according to the amount of multipartite entanglement they posses. Here, $y_i = 1$ if the states posses a large amount of multipartite entanglement (according to some measure), while $y_i = 0$ if the states are separable. Since local unitaries do not change the multipartite entanglement in a quantum state, then we have that $f((\bigotimes_j^n U_j)\rho_i(\bigotimes_j^n U_j^\dagger)) = f(\rho_i)$ for any local unitary U_j acting on the j-th qubit.

- *States:* Pure states $\rho_i \in \mathcal{D}(\mathcal{H})$
- *Labels:* $y_i \in [0, 1]$, where 0 means separable and 1 means "highly entangled"
- *Group:* $G = U(2) \times \cdots \times U(2)$, ($n$ times)
- *Representation:* $U : G \mapsto U(d)$, where $(g_1, \ldots, g_n) \cdot \rho_i = (U_{g_1} \otimes \cdots \otimes U_{g_n})\rho_i(U_{g_1} \otimes \cdots \otimes U_{g_n})^\dagger$

Figure 7.25:

Chapter 8

Perturbation Theory

Say you have some system H of an n particle system and want to calculate its eigenspectrum (i.e. its eigenvalues and eigenstates) or the dynamics it induces. In certain cases this is easy - e.g., if the n particles are non-interacting, if we can identify its symmetries to Block diagonalize the Hamiltonian or if we can apply physics intuition to transform into some other clever basis where diagonalizing the Hamiltonian is easy. But generally this is hard and we need to resort to approximation techniques.

Perturbation theory is an approach to handling complex Hamiltonians by breaking up the Hamiltonian into 'easier' terms that you know how to diagonalize and small corrections that we can treat as inducing perturbative corrections. Exactly, how to do this in practise depends on whether there is or isn't a time dependence, whether there is or isn't degeneracy in the eigenstates, as well as the available computational power. Let's start with the simple non-degenerative time-independent case.

8.1 Non-degenerate Time-Independent Perturbation Theory

Let's consider a physical problem governed by a Hamiltonian $\hat{H}$, which we decompose as

$$\hat{H} = \hat{H}_0 + \lambda\hat{V} \tag{8.1}$$

where $\hat{H}_0$ is a Hamiltonian with known eigenenergies and eigenstates (i.e. its the easy part), $\lambda \in \mathbb{R}^+$ is a real positive parameter determining the strength of the additional term $\hat{V}$ which is

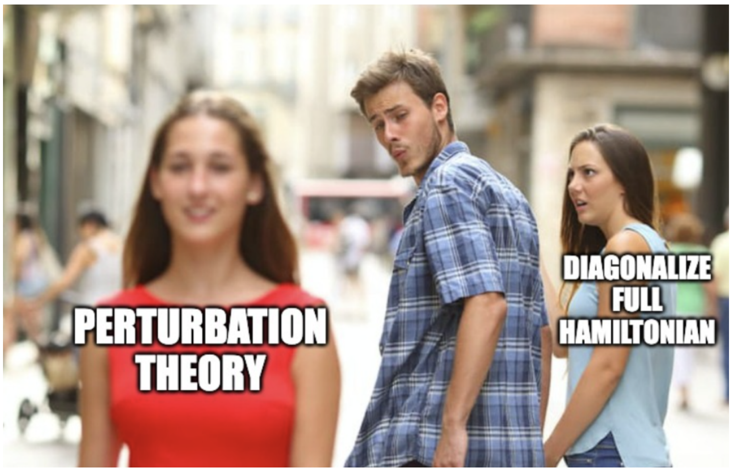


Figure 8.1: Caption

treated as a *perturbation* of the system. We are interested in studying the limit of this problem where λ is small (i.e., the limit of small perturbations).

Let $|\phi_n\rangle$ denote the *known* eigenstates of $\hat{H}_0$ and ϵ_n the associated eigenenergies. The goal of this section is to establish techniques to determine the eigenenergies of the total Hamiltonian $\hat{H}$. For sufficiently small perturbations λ, it is reasonable to assume that the eigenstates $|\psi_n\rangle$ of $\hat{H}$ will be "close" to $|\phi_n\rangle$, and the associated energies E_n will be close to ϵ_n. In the limit of very small λ, the solution can be expanded in powers of λ:

$$|\psi_n\rangle = |\phi_n\rangle + \lambda\,|\psi_n^{(1)}\rangle + \lambda^2\,|\psi_n^{(2)}\rangle + \cdots \tag{8.2}$$

$$E_n = \epsilon_n + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \cdots. \tag{8.3}$$

And Schrödinger equation is written as:

$$\begin{aligned}\left(\hat{H}_0 + \lambda\hat{V}\right)&\left(|\phi_n\rangle + \lambda\,|\psi_n^{(1)}\rangle + \lambda^2\,|\psi_n^{(2)}\rangle + \cdots\right)\\ &= \left(\epsilon_n + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \cdots\right)\left(|\phi_n\rangle + \lambda\,|\psi_n^{(1)}\rangle + \lambda^2\,|\psi_n^{(2)}\rangle + \cdots\right).\end{aligned} \tag{8.4}$$

Our goal is to find explicit expressions for the perturbations to the eigenstates $|\psi_n^{(k)}\rangle$ and corrections to the eigenenergies $E_n^{(k)}$ for $k = 1, 2, ...$

The equation 8.4 must be satisfied at each order in λ. This allows us to iteratively identify the corrections $E_n^{(k)}$ and $|\psi_m^{(k)}\rangle$.

Zero-th Order. At order 0 we simply have the unperturbed eigenvalue problem:

$$\hat{H}_0\,|\phi_n\rangle = \epsilon_n\,|\phi_n\rangle\,.$$

1st Order. At order 1 we have:

$$\hat{H}_0\,|\psi_n^{(1)}\rangle + \hat{V}\,|\phi_n\rangle = \epsilon_n\,|\psi_n^{(1)}\rangle + E_n^{(1)}\,|\phi_n\rangle\,,\,. \tag{8.5}$$

To isolate the first order correction to the eigenenergy, $E_1^{(1)}$, we can bra through with $\langle\phi_n|$:

$$\langle\phi_n|\hat{H}_0|\psi_n^{(1)}\rangle + \langle\phi_n|\hat{V}|\phi_n\rangle = \epsilon_n\langle\phi_n|\psi_n^{(1)}\rangle + E_n^{(1)}\underbrace{\langle\phi_n|\phi_n\rangle}_{=1} \tag{8.6}$$

$$\epsilon_n\langle\phi_n|\psi_n^{(1)}\rangle + \langle\phi_n|\hat{V}|\phi_n\rangle = \epsilon_n\langle\phi_n|\psi_n^{(1)}\rangle + E_n^{(1)} \tag{8.7}$$

where in the second line we have used $\hat{H}_0\,|\phi_0\rangle = \epsilon_0\,|\phi_0\rangle$. We therefore find that the first order correction to the energy of $\hat{H}_0$ due to $\hat{V}$ is given by:

$$E_n^{(1)} = \langle\phi_n|\hat{V}|\phi_n\rangle \tag{8.8}$$

and so the eigenenergies of H to 1st order are:

$$E_n = \epsilon_n + \lambda\,\langle\phi_n|\hat{V}|\phi_n\rangle + \mathcal{O}(\lambda^2) \tag{8.9}$$

What about the first order correction to the eigenstate? Our goal will be to write the correction in the basis of the original eigenstates:

$$|\psi_n^{(1)}\rangle = \sum_m\langle\phi_m|\psi_n^{(1)}\rangle|\phi_m\rangle\,. \tag{8.10}$$

Thus we need to compute the overlaps $\langle\phi_m|\psi_n^{(1)}\rangle$. To do this we start with Eq. (8.5) but instead bra through with $\langle\phi_m|$. This gives

$$\langle\phi_m|\hat{H}_0|\psi_n^{(1)}\rangle + \langle\phi_m|\hat{V}|\phi_n\rangle = \epsilon_n\langle\phi_m|\psi_n^{(1)}\rangle + E_n^{(1)}\underbrace{\langle\phi_m|\phi_n\rangle}_{=0} \tag{8.11}$$

$$\epsilon_m\langle\phi_m|\psi_n^{(1)}\rangle + \langle\phi_m|\hat{V}|\phi_n\rangle = \epsilon_n\langle\phi_m|\psi_n^{(1)}\rangle \tag{8.12}$$

which can be rearranged to give:

$$\langle\phi_m|\psi_n^{(1)}\rangle = \frac{\langle\phi_m|\hat{V}|\phi_n\rangle}{\epsilon_n - \epsilon_m}\,. \tag{8.13}$$

This looks promising but what is going on for $m = n$? To understand this remember that $\{|\psi_n\rangle\}$ are the eigenbasis of $\hat{H}$ and so form a normalised eigenbasis with

$$\langle\psi_n|\psi_{n'}\rangle = \delta_{n,n'}\,. \tag{8.14}$$

For $n = n$ this constraint can be rewritten to first order in λ as

$$1 = \langle\psi_n|\psi_n\rangle = \langle\phi_n|\phi_n\rangle + \lambda(\langle\phi_n|\psi_n^{(1)}\rangle + \langle\psi_n^{(1)}|\phi_n\rangle) + \mathcal{O}(\lambda^2)\,. \tag{8.15}$$

As λ is positive we therefore have that:

$$\langle\phi_n|\psi_n^{(1)}\rangle + \langle\psi_n^{(1)}|\phi_n\rangle = 2\mathfrak{Re}(\langle\psi_n^{(1)}|\phi_n\rangle) = 0\,. \tag{8.16}$$

We are free to choose the global (unphysical) phase of the original eigenstates $|\phi_n\rangle$ such that $\langle\psi_n^{(1)}|\phi_n\rangle$ is purely real. Thus we end up with

$$\langle\phi_n|\psi_n^{(1)}\rangle = \langle\psi_n^{(1)}|\phi_n\rangle = 0\,. \tag{8.17}$$

Putting this all together we have that

$$|\psi_n^{(1)}\rangle = \sum_{m\neq n}\frac{\langle\phi_m|\hat{V}|\phi_n\rangle}{\epsilon_n - \epsilon_m}|\phi_m\rangle \tag{8.18}$$

and so the eigenstates of $\hat{H}$ to 1st order are:

$$|\psi_n\rangle = |\phi_n\rangle + \lambda|\psi_n^{(1)}\rangle + \mathcal{O}(\lambda^2) = |\phi_n\rangle + \lambda\sum_{m\neq n}\frac{\langle\phi_m|\hat{V}|\phi_n\rangle}{\epsilon_n - \epsilon_m}|\phi_m\rangle + \mathcal{O}(\lambda^2)\,. \tag{8.19}$$

2nd Order. At order 2 we have:

$$\hat{H}_0\,|\psi_n^{(2)}\rangle + \hat{V}\,|\psi_n^{(1)}\rangle = \epsilon_n\,|\psi_n^{(2)}\rangle + E_n^{(1)}\,|\psi_n^{(1)}\rangle + E_n^{(2)}\,|\phi_n\rangle\,. \tag{8.20}$$

To get the second order energy correction we can again bra through with $\langle\phi_n|$ which gives:

$$\epsilon_n\langle\phi_n|\psi_n^{(2)}\rangle + \langle\phi_n|\hat{V}\,|\psi_n^{(1)}\rangle = \epsilon_n\langle\phi_n|\psi_n^{(2)}\rangle + E_n^{(1)}\langle\phi_n|\psi_n^{(1)}\rangle + E_n^{(2)}\,. \tag{8.21}$$

On cancelling terms, recalling that $\langle\phi_n|\psi_n^{(1)}\rangle = 0$ and substituting in Eq. (8.18), this gives:

$$E_n^{(2)} = \langle\phi_n|\hat{V}|\psi_n^{(1)}\rangle = \sum_{m\neq n}\frac{\langle\phi_m|\hat{V}|\phi_n\rangle}{\epsilon_n - \epsilon_m}\langle\phi_n|\hat{V}|\phi_m\rangle = \sum_{m\neq n}\frac{|\langle\phi_m|\hat{V}|\phi_n\rangle|^2}{\epsilon_n - \epsilon_m}\,. \tag{8.22}$$

For the second order correction to the eigenstate things start to become messy but you can keep on iterating this procedure to obtain an explicit expression for the eigenstates to second order. You'll be pleased to know I won't make you do this in this course.

Comment 1. The above calculation implicitly assumed that the energy levels are non-degenerate. If you have degenerate eigenvalues (i.e. two different eigenstates with the same energy) then the denominator in Eq. (8.18) blows up. We will come back to how to deal with this case later in this section.

Comment 2. For this approximation to be valid we need the second order correction to be small compared to the first order correction. How can we check this? To derive one way of checking let Δ be the energy difference between ϵ_n and the nearest energy level i.e. $\Delta = \min_m |\epsilon_n - \epsilon_m|$. Then we can write:

$$\begin{aligned}
\left|E_n^{(2)}\right| &= \Big|\sum_{m\neq n} \frac{\left|\langle\phi_m|\hat{V}|\phi_n\rangle\right|^2}{(\epsilon_n-\epsilon_m)}\Big| \\
&\leq \sum_{m\neq n} \frac{\left|\langle\phi_m|\hat{V}|\phi_n\rangle\right|^2}{|\epsilon_n-\epsilon_m|} \\
&\leq \frac{1}{\Delta}\sum_{m\neq n} \left|\langle\phi_m|\hat{V}|\phi_n\rangle\right|^2 \\
&= \frac{1}{\Delta}\left(\sum_m \langle\phi_n|\hat{V}|\phi_m\rangle\langle\phi_m|\hat{V}|\phi_n\rangle - \left|\langle\phi_n|\hat{V}|\phi_n\rangle\right|^2\right) \\
&= \frac{1}{\Delta}\left(\langle\phi_n|\hat{V}^2|\phi_n\rangle - \langle\phi_n|\hat{V}|\phi_n\rangle^2\right).
\end{aligned}$$

The condition $|E_n^{(2)}| \ll |E_n^{(1)}|$ is satisfied as long as,

$$\frac{1}{\Delta}\left(\langle\phi_n|\hat{V}^2|\phi_n\rangle - \langle\phi_n|\hat{V}|\phi_n\rangle^2\right) \ll \langle\phi_n|\hat{V}|\phi_n\rangle\ , \tag{8.23}$$

or equivalently, as long as:

$$\left|\frac{\langle\phi_n|\hat{V}^2|\phi_n\rangle}{\langle\phi_n|\hat{V}|\phi_n\rangle} - \langle\phi_n|\hat{V}|\phi_n\rangle\right| \ll \Delta\,. \tag{8.24}$$

A more restrictive but also easier-to-verify condition would be to require that the elements of the perturbation matrix are small compared to the energy level spacing. In other words, we impose:

$$\left|\frac{\langle\phi_m|\hat{V}|\phi_n\rangle}{\epsilon_n-\epsilon_m}\right| \ll 1.$$

8.1.1 Examples

Example 8.1.1. **Harmonic Oscillator Exposed to a Constant Force.** Suppose we consider particle in a Harmonic well subject to a constant force:

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2x^2 - qEx\,. \tag{8.25}$$

We can write this Hamiltonian as $H = H_0 + \lambda V$ with

$$\begin{aligned}
H_0 &= \frac{p^2}{2m} + \frac{1}{2}m\omega^2x^2 \\
V &= -qEx
\end{aligned} \tag{8.26}$$

and $\lambda = 1$. We know the energies of H_0, as this is just the simple harmonic oscillator with energies

$$\epsilon_n = \hbar\omega\left(n + \frac{1}{2}\right) \tag{8.27}$$

and eigenstates $|n\rangle$. To simplify things, we express V using the lowering and raising operators

$$V = -qEx = -qE\sqrt{\frac{\hbar}{2m\omega}}(a + a^\dagger) \tag{8.28}$$

with $a|n\rangle = \sqrt{n}|n-1\rangle$ and $a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$. To find the 1st order corrections to the energies, we use $E_n^{(1)} = \langle n|V|n\rangle$:

$$E_n^{(1)} = -qE\sqrt{\frac{\hbar}{2m\omega}}\langle n|(a + a^\dagger)|n\rangle = 0 \tag{8.29}$$

and thus the first order correction to the energy vanishes [1].

To find the 2nd order corrections to the energies, we write

$$\begin{aligned} E_n^{(2)} &= \sum_{m\neq n} \frac{|\langle m|V|n\rangle|^2}{\epsilon_n - \epsilon_n} && (8.30)\\ &= \frac{q^2E^2\hbar}{2m\omega}\sum_{m\neq n}\frac{|\langle m|(a+a^\dagger)|n\rangle|^2}{\hbar\omega(n-m)} && (8.31)\\ &= \frac{q^2E^2}{2m\omega^2}\sum_{m\neq n}\frac{|\langle m|(a+a^\dagger)|n\rangle|^2}{(n-m)}\,. && (8.32) \end{aligned}$$

To simplify this we use the fact that $a|n\rangle = \sqrt{n}|n-1\rangle$ and $a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$ to find

$$\begin{aligned} E_n^{(2)} &= \frac{q^2E^2\hbar}{2m\omega}\sum_{m\neq n}\frac{|\sqrt{n}\langle m|n-1\rangle + \sqrt{n+1}\langle m|n+1\rangle|^2}{\hbar\omega(n-m)} && (8.33)\\ &= \frac{q^2E^2}{2m\omega^2}\left(\frac{|\sqrt{n}|^2}{n-(n-1)} + \frac{|\sqrt{n+1}|^2}{n-(n+1)}\right) && (8.34)\\ &= -\frac{q^2E^2}{2m\omega^2} && (8.35) \end{aligned}$$

So, up to second order, we have

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right) - \frac{q^2E^2}{2m\omega^2}\,. \tag{8.36}$$

Note that for this simple example you can just solve this Hamiltonian exactly by seeing that a constant force simply shifts the equilibrium position (the position where the force vanishes) to $x_0 = qE/(m\omega^2)$ as

$$\begin{aligned} H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2x^2 - qEx &= \frac{p^2}{2m} + \frac{1}{2}m\omega^2\left(x - \frac{qE}{m\omega^2}\right)^2 - \left(\frac{qE}{m\omega^2}\right)^2\\ &= \frac{p^2}{2m} + \frac{1}{2}m\omega^2\left(x - x_0\right)^2 - \frac{1}{2}m\omega^2x_0^2\,. \end{aligned} \tag{8.37}$$

Thus you can see that the perturbation reduces the energy by $\frac{1}{2}m\omega^2x_0^2 = \frac{q^2E^2}{2m\omega^2}$. We therefore see that in this case 2nd order perturbation theory gives us the exact values of energies for the Hamiltonian. However, this is is only true for this simple example and not generally the case.

[1] An alternative way of seeing this would be to note that $|n\rangle$ are even under reflections $x \to -x$ but x is of course odd and the above equation corresponds to integrating an odd function for $x = -\infty$ to $x = \infty$.

Example 8.1.2. **Potential of a Diatomic Molecule.** Consider the following Hamiltonian $\hat{H} = \hat{H}_0 + \hat{V}$ with:

$$\begin{cases} \hat{H}_0 = \frac{\hat{p}^2}{2} + \frac{\hat{x}^2}{2}, \\ \hat{V} = c\hat{x}^3 + q\hat{x}^4, \end{cases}$$

for $c \geq 0$ and $q \leq 0$. Note that to make our life less miserable here we have picked units such that $\hbar\omega = m = 1$ (in contrast to the previous example).

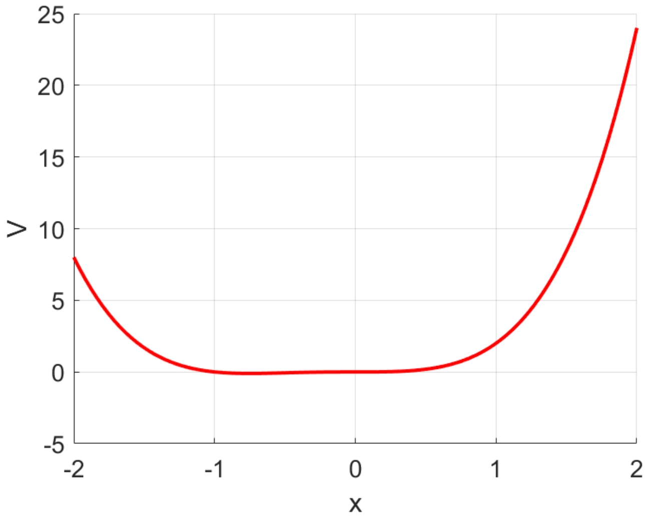


Figure 8.2: Correction to the potential

The energy and eigenstates of $\hat{H}_0$ for the system are already known- this is just a standard quantum harmonic oscillator. Concretely, we have $\epsilon_n = (n + \frac{1}{2})$. The goal is to determine the $E_n^{(k)}$ for a fixed n. From Eq. (8.9) the first order correction to the eigenenergies is given by:

$$E_n^{(1)} = \langle n|c\hat{x}^3 + q\hat{x}^4|n\rangle \, .$$

To evaluate this let's introduce creation and annihilation operators such that $\hat{x} = \hat{a} + \hat{a}^\dagger$. It is immediately noticed that the term $c\hat{x}^3$ does not contribute because only terms with the same number of $\hat{a}^\dagger$ and $\hat{a}$ operators give rise to non-zero coefficients (alternatively, note that the eigenstates $|n\rangle$ are symmetric under $\hat{x} \to -\hat{x}$). Next we note that:

$$\begin{aligned} \hat{x}^4 &= \left(\hat{a} + \hat{a}^\dagger\right)^4 = \left((\hat{a})^2 + \hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a} + \hat{a}^{\dagger 2}\right)^2 \\ &= (\hat{a})^4 + (\hat{a})^2\hat{a}^{\dagger 2} + (\hat{a})^3\hat{a}^\dagger + (\hat{a})^2\hat{a}^\dagger\hat{a} \\ &+ \hat{a}^{\dagger 2}(\hat{a})^2 + \hat{a}^{\dagger 4}\hat{a}^{\dagger 2}\hat{a}\hat{a}^\dagger + \hat{a}^{\dagger 3}\hat{a} + \hat{a}\hat{a}^\dagger(\hat{a})^2 \\ &+ \hat{a}\hat{a}^{\dagger 3} + \hat{a}\hat{a}^\dagger\hat{a}\hat{a}^\dagger + \hat{a}\hat{a}^\dagger\hat{a}^\dagger\hat{a} + \hat{a}^\dagger(\hat{a})^3 \\ &+ \hat{a}^\dagger\hat{a}\hat{a}^{\dagger 2} + \hat{a}^\dagger\hat{a}\hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a}\hat{a}^\dagger\hat{a} \\ &= (\hat{a})^2\,\hat{a}^{\dagger 2} + \hat{a}^{\dagger 2}\,(\hat{a})^2 + \hat{a}\hat{a}^\dagger\hat{a}^\dagger\hat{a} + \hat{a}^\dagger\hat{a}\hat{a}\hat{a}^\dagger + \hat{a}\hat{a}^\dagger\hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a}\hat{a}^\dagger\hat{a}, \end{aligned}$$

where the last equality is obtained by again noting that only terms with equal numbers of creation and annihilation operators lead to non-zero contributions. Thus (after a bunch of algebra which I will leave it up to you to fill in) we find:

$$\langle n|\left(\hat{a}^\dagger + \hat{a}\right)^4|n\rangle = \langle n|\,(\hat{a})^2\,\hat{a}^{\dagger 2}|n\rangle + \langle n|\hat{a}^{\dagger 2}\,(\hat{a})^2\,|n\rangle + \langle n|\hat{a}\hat{a}^\dagger\hat{a}^\dagger\hat{a}|n\rangle + \langle n|\hat{a}^\dagger\hat{a}\hat{a}\hat{a}^\dagger|n\rangle + \langle n|\hat{a}\hat{a}^\dagger\hat{a}\hat{a}^\dagger|n\rangle + \langle n|\hat{a}^\dagger\hat{a}\hat{a}^\dagger\hat{a}|n\rangle \quad =$$

And so we have

$$\epsilon_n \approx \left(n + \frac{1}{2}\right) - 6|q|\left(n^2 + n - \frac{1}{2}\right) . \tag{8.38}$$

8.2 Degenerate Time-Independent Perturbation Theory

As mentioned earlier, the approach described above fails when $\hat{H}_0$ has degenerate eigenvalues because of terms of the form $\frac{1}{\epsilon_n - \epsilon_m} = \frac{1}{0}$ in Eq. (8.18). In this section we show how we can deal with this case.

For simplicity, we assume for now that only for the n_{th} energy state is there an N-fold degeneracy. That is, we suppose that the initial Hamiltonian H_0 has energy ϵ_n with N degenerate states ϕ_{n_i}, $i = 1, \ldots, N$.

Let us start by finding the first order corrections $E_n^{(1)}$. To do so, we expand our eigenstate $|\psi_n\rangle$ in powers of λ. However, this time we replace the 0-th order term $|\phi_n\rangle$ with a linear combination $\sum_j c_j |\phi_{n_j}\rangle$ of the degenerate states because we are unsure of what combination of these states yields the "correct" 0-th order contribution to $|\psi_n\rangle$. That is, we can write:

$$|\psi_n\rangle = \sum_j c_j |\phi_{n_j}\rangle + \lambda|\psi_n^{(1)}\rangle + \lambda^2|\psi_n^{(2)}\rangle + \ldots \tag{8.39}$$

and the energy is given by

$$E_n = \epsilon_n + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \ldots \tag{8.40}$$

as previously. Again, working from the Schrödinger equation $H|\psi_n\rangle = E_n|\psi_n\rangle$ to first order in λ we have:

$$H_0|\psi_n^{(1)}\rangle + \sum_j c_j V|\phi_{n_j}\rangle = \epsilon_n|\psi_n^{(1)}\rangle + E_n^{(1)} \sum_j c_j|\phi_{n_j}\rangle$$

Similarly to the non-degenerate case we next bra through with $\langle\phi_{n_i}|$,

$$\langle\phi_{n_i}|H_0|\psi_n^{(1)}\rangle + \sum_j c_j\langle\phi_{n_i}|V|\phi_{n_j}\rangle = \epsilon_n\langle\phi_{n_i}|\psi_n^{(1)}\rangle + E_n^{(1)} \sum_j c_j\langle\phi_{n_i}|\phi_{n_j}\rangle$$

and cancel the ϵ_n terms to give:

$$\sum_j \langle\phi_{n_i}|V|\phi_{n_j}\rangle c_j = E_n^{(1)} \sum_j c_j\langle\phi_{n_i}|\phi_{n_j}\rangle = E_n^{(1)} \sum_j c_j\delta_{ij} = E_n^{(1)} c_i$$

The terms $\langle\phi_{n_i}|V|\phi_{n_j}\rangle = V_{ij}$ are the matrix elements of V in the $\{|\phi_{n_i}\rangle\}$ basis of degenerate 0-th order states. Thus we have:

$$\sum_j V_{ij} c_j = E_n^{(1)} c_i$$

This is precisely an eigenvalue equation. The first order corrections $E_n^{(1)}$ are the eigenvalues of V in the degenerate state basis and the corresponding vectors c_i characterize the "correct" linear combination $\sum_j c_j|\phi_{n_j}\rangle$ in the 0-th order term of the eigenstate $|\psi_n\rangle$.

Finding eigenvalues and eigenvectors of a matrix are equivalent to diagonalizing it - so, when we carry about this procedure for finding the 1st order corrections to the energies of degenerate states, we just diagonalize the perturbation Hamiltonian V.

Comment 1. Note that in the context of perturbation theory for a non-degenerate physical system, the perturbation appears at order 1 in λ, while here we have a correction to the zero-th order state.

Comment 2. In general, a perturbation allows us to *lift degeneracy*, i.e., obtain energy corrections $E_{n,i}^{(1)}$ that are all different. Any remaining degeneracies are actually due to intrinsic symmetries, directly related to the physics of the problem. This links back to the previous comment - it is because the degeneracy is lifted that the 0th order contribution changes.

8.2.1 Examples

Example 8.2.1. **Trivial example.** We first note that this approach trivially works for the case of a Hamiltonian $H = H_0 + V$ with $H_0 = aI$. In this case eigenstates of H_0 are trivially degenerate and the eigenvalues and eigenvectors of the perturbed Hamiltonian can be found by finding the eigenvalues and eigenvectors of the perturbation V.

Example 8.2.2. **The Stark Effect.** The Stark effect is an important phenomenon in atomic physics where one observes the splitting of the degeneracy of one-electron atoms in an electric field. In this example we consider the Hamiltonian of a one-electron atom (e.g. Hydrogen) in a constant, uniform electric field E which points only in the z direction. We neglect spin in this example. (If you can't remember the physics of the hydrogen atom now is a good moment to recap it!) The Hamiltonian of such a system is

$$H = \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + \frac{p_z^2}{2m} - \frac{e^2}{4\pi\epsilon_0 r} - e\mathcal{E}z = H_0 + V$$

where V is identified with the term $-e\mathcal{E}z$. The n_{th} energy eigenvalue of the unperturbed Hamiltonian is n^2-fold degenerate. In this example, we will consider the case of $n = 2$, which has a 4-fold degeneracy; the corresponding degenerate eigenstates are given in $|nlm\rangle$ notation by $|200\rangle$, $|211\rangle$, $|210\rangle$, $|21-1\rangle$.

To find the 0th order correction to the eigenstate and 1st order contribution to the eigenenergy we need to diagonalize V in the eigen-space spanned by $|200\rangle$, $|211\rangle$, $|210\rangle$, $|21-1\rangle$. I.e., we need to find the eigenvalues and eigenvectors of:

$$\tilde{V} = \begin{bmatrix} (200|V|200) & (200|V|210) & (200|V|211) & (200|V|21-1) \\ (210|V|200) & (210|V|210) & (210|V|211) & (210|V|21-1) \\ (211|V|200) & (211|V|210) & (211|V|211) & (211|V|21-1) \\ (21-1|V|200) & (21-1|V|210) & (21-1|V|211) & (21-1|V|21-1) \end{bmatrix} \tag{8.41}$$

This looks like a nasty thing to work with but luckily it turns out most of the terms are zero. Each of the 16 matrix elements is of the form:

$$V_{lm,l'm'} = \langle 2,l,m|z|2,l',m'\rangle = \iiint u_{lm}^*(r\cos\theta)u_{l'm'}r^2\sin\theta d\theta d\phi dr \tag{8.42}$$

where we recall that

$$\begin{aligned} u_{00} &\propto \left(1 - \frac{r}{2a_0}\right)e^{-r/2a_0} \\ u_{10} &\propto r\cos\theta e^{-r/2a_0} \\ u_{11} &\propto r\sin\theta e^{i\phi}e^{-r/2a_0} \\ u_{1-1} &\propto r\sin\theta e^{-i\phi}e^{-r/2a_0} \end{aligned} \tag{8.43}$$

where a_0 is the Bohr radius. Looking first at parity, it is clear that $z = r\cos(\theta)$ has odd parity. And thus any term along the diagonal is the integral over an odd function and so is zero. Similar parity arguments apply for $V_{1-1,11}$ terms. Secondly, $\int_0^{2\pi} e^{i\phi}d\phi = 0$, so any term with a single u_{11}

or u_{1-1} contribution vanishes, e.g. $V_{00,1-1} = V_{11,00} = V_{1-1,00} = 0$. Thus we end up with only two non-zero terms corresponding to $V_{00,01}$. Thus we have left with:

$$\tilde{V} = \begin{bmatrix} 0 & \alpha & 0 & 0 \\ \alpha^* & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

where (if you do the integrals) $\alpha = -3e\mathcal{E}a_0$. It is now easy to see[2] that the eigenvalues of $\tilde{V}$ are $\pm 3e\mathcal{E}a_0$ and 0. The corresponding eigenkets are $2^{-1/2}(1, \pm 1, 0, 0)$, $(0, 0, 1, 0)$ and $(0, 0, 0, 1)$ (with the final two eigenstates still degenerate). We conclude that as soon as the slightest perturbation is switched on, the system is in the state of lowest energy, i.e.,

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|200\rangle + |210\rangle) \tag{8.44}$$

with energy $E_b = -3a_0 e\mathcal{E}$.

[2]The top left hand block just corresponds to diagonalizing σ_x, and the lower block is just the all zero matrix.

Chapter 9

Time-dependent Hamiltonians

So far, we have focused on approximating the eigenstates and eigenvalues of systems described by time-independent Hamiltonians. What happens when we can no longer neglect time dependence? We want to solve the equation:

$$i\frac{\partial}{\partial t}|\phi(t)\rangle = \hat{H}(t)|\phi(t)\rangle. \tag{9.1}$$

Equivalently, we can always write

$$|\phi(t)\rangle = \hat{U}(t,t_0)|\phi(t_0)\rangle. \tag{9.2}$$

for some unitary $\hat{U}(t,t_0)$. If the Hamiltonian is time-independent, it has the form

$$\hat{U}(t,t_0) = e^{-i\hat{H}(t-t_0)}, \tag{9.3}$$

but when there is explicit time dependence we cannot use this simple expression. This chapter will be give you some tools for computing the propagator in this case.

We will start by deriving something call the 'Dyson series'. This gives an exact expression for the evolution operator of a quantum system with a time dependent Hamiltonian. Unfortunately this expression is in most cases so disgustingly messy that you can not do much with it. We will then explore the interaction representation which (partially) simplifies the picture. Finally, we will go back to perturbation theory (this time 'time-dependent perturbation theory') to show that if the time dependent part of the Hamiltonian is only a small perturbation then calculations again become nice and tractable.

9.1 Dyson series

I warn you that this is a slightly fiddly derivation - but it's one of those derivations everyone needs to see at least once.

Plugging our expression for the evolution operator, Eq. (9.2), into the Schrodinger equation, Eq. (9.1), we have

$$i\frac{\partial}{\partial t}\hat{U}(t,t_0)|\phi(t_0)\rangle = \hat{H}(t)|\phi(t)\rangle. \tag{9.4}$$

As this holds for any state we thus have

$$\begin{cases} i\frac{\partial}{\partial t}\hat{U}(t,t_0) = \hat{H}(t)\hat{U}(t,t_0), \\ \hat{U}(t_0,t_0) = \mathbb{1}. \end{cases} \tag{9.5}$$

The exact time evolution operator in the case of a time dependent Hamiltonian is obtained by solving this system of equations. Integrating the first equation from t_0 to t gives:

$$\begin{aligned} i\int_{t_0}^{t} dt_1 \frac{\partial}{\partial t}\hat{U}(t_1,t_0) &= \int_{t_0}^{t} dt_1 \hat{H}(t_1)\hat{U}(t_1,t_0) \\ \Longrightarrow i\left(\hat{U}(t,t_0) - \mathbb{1}\right) &= \int_{t_0}^{t} dt_1 \hat{H}(t_1)\hat{U}(t_1,t_0). \end{aligned}$$

Therefore,

$$\begin{aligned} \hat{U}(t,t_0) &= \mathbb{1} - i\int_{t_0}^{t} dt_1 \hat{H}(t_1)\hat{U}(t_1,t_0) \\ &= \mathbb{1} - i\int_{t_0}^{t} dt_1 \hat{H}(t_1)\left(\mathbb{1} - i\int_{t_0}^{t_1} dt_2 \hat{H}(t_1)\hat{U}(t_2,t_0)\right) \\ &= \mathbb{1} - i\int_{t_0}^{t} dt_1 \hat{H}(t_1) + (-i)^2\int_{t_0}^{t} dt_1\int_{t_0}^{t_1} dt_2 \hat{H}(t_1)\hat{H}(t_2)\hat{U}(t_2,t_0) \\ &= \mathbb{1} + \sum_{n=1}^{\infty}(-i)^n\int_{t_0}^{t} dt_1\int_{t_0}^{t_1} dt_2 \cdots \int_{t_0}^{t_{n-1}} dt_n \hat{H}(t_1)\hat{H}(t_2)\hat{H}(t_3)\cdots\hat{H}(t_n) \end{aligned} \tag{9.6}$$

where $t_i > t_{i-1}$ for all i. (Note that the final $U(t_n,t_0)$ term vanishes, i.e, becomes an identity, in the limit that $n \to \infty$.)

This looks pretty messy and hard to work with. In particular, its a pain how each of the integrals range depend on other parameters we are integrating over. It would be much nicer if all the integrals were between t_0 and t. To do so [1], we will need to introduce the *time ordering operator*, T. This is defined as follows:

$$T\left[H(t_1)H(t_2)\cdots H(t_n)\right] = H(t_{i_1})H(t_{i_2})\cdots H(t_{i_n}), \quad \text{where} \quad t_{i_1} > t_{i_2} > \cdots > t_{i_n}\,. \tag{9.7}$$

That is, the time-ordering operator tells you to reorder the operators so the time arguments of the corresponding operators *decrease* as you go moves from the left to the right. You end up with an expression where the largest time appears in the argument of the first (left most) operator and the smallest time appears in the argument of the last (right most) operator. For example, if $t_2 > t_1$ then you have

$$T(H(t_1)H(t_2)) = H(t_2)H(t_1)\,. \tag{9.8}$$

Ok, so how does this help to simplify Eq. (9.6)? To see how let's look at the term:

$$J_2 = \int_{t_0}^{t} dt_1\int_{t_0}^{t_1} dt_2 \hat{H}(t_1)\hat{H}(t_2) \text{ with } t_2 \le t_1\,. \tag{9.9}$$

In this expression the integration over t_2 is performed first from t_0 to t_1, and then t_1 is integrated from t_0 to t. This represents all the pairs (t_1,t_2) where $t_2 \le t_1 \le t$. Geometrically, we can visualise this as looking for the area of the shaded area in Fig. 9.1(a). Now, as $t_2 \le t_1$ we have $T\left[H(t_1)H(t_2)\right] = H(t_1)H(t_2)$ and so we are free to insert T into the above integral to give

$$J_2 = \int_{t_0}^{t} dt_1\int_{t_0}^{t_1} dt_2 \hat{H}(t_1)\hat{H}(t_2) = \int_{t_0}^{t} dt_1\int_{t_0}^{t_1} dt_2 T\left[H(t_1)H(t_2)\right] \tag{9.10}$$

Next, we are free to change the order of integration (this is equivalent to integrating over the shaded region in Fig. 9.1(b) which is the same as the region in (a)). Thus we have

$$J_2 = \int_{t_0}^{t} dt_1\int_{t_0}^{t_1} dt_2 H(t_1)H(t_2) = \int_{t_0}^{t} dt_2\int_{t_2}^{t} dt_1 H(t_1)H(t_2). \tag{9.11}$$

[1] In places here I am directly copying from these notes- you may prefer to go and read the original.

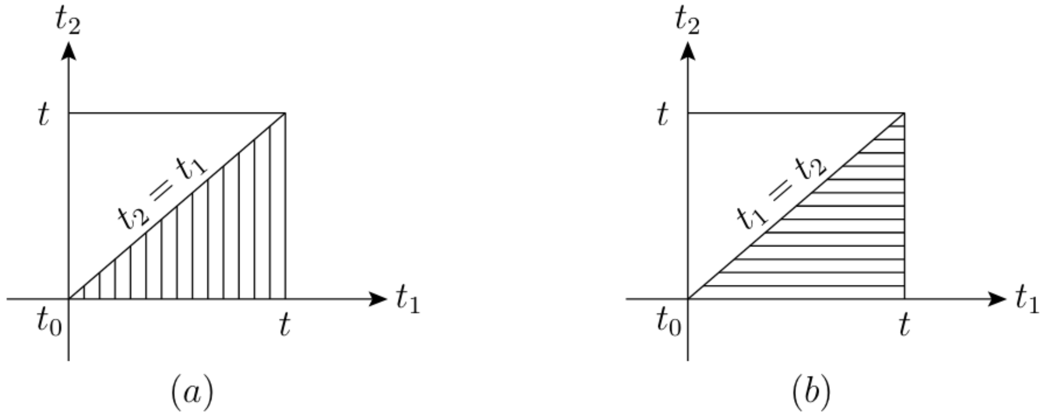


Figure 9.1: The integration region, $t_0 \leq t_1 \leq t$ and $t_0 \leq t_2 \leq t_1$, used in Eq. (9.10) (b) The integration region, $t_0 \leq t_2 \leq t$ and $t_2 \leq t_1 \leq t$, employed in Eq. (9.11) after interchanging the order of integration. (Image from this nice set of notes on the Dyson series.)

As the integration variables, t_1 and t_2, are dummy labels, we can relabel the integration variables in the final expression in Eq. (9.11) with by $t_1 \to t_2$ and $t_2 \to t_1$ to give:

$$J_2 = \int_{t_0}^{t} dt_1 \int_{t_1}^{t} dt_2 H(t_2) H(t_1) = \int_{t_0}^{t} dt_1 \int_{t_1}^{t} dt_2 T\left[H(t_1)H(t_2)\right]. \tag{9.12}$$

In the second equality we have inserted the T symbol. As now $t_2 \geq t_1$ (after the relabelling), in this case we have $T\left[H(t_1)H(t_2)\right] = H(t_2)H(t_1)$. That is, the integration region now consists of the area of the half square above the diagonal line shown in Fig. 9.1(a).

We now have two different expressions for J_2,

$$J_2 = \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 T\left[H(t_1)H(t_2)\right] = \int_{t_0}^{t} dt_1 \int_{t_1}^{t} dt_2 T\left[H(t_1)H(t_2)\right]. \tag{9.13}$$

Therefore, $2J_2$ is equal to the sum of the two integrals given in Eq. (9.13). By adding the two integrals, the dependence on the integration limit t_1 disappears. The integration region is now the area bounded by the full square. After dividing by two, we end up with,

$$J_2 = \frac{1}{2} \int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 T\left[H(t_1)H(t_2)\right]. \tag{28}$$

That is, we have successfully decoupled the limits.

Iterating this procedure, you find that the time evolution operator can be written in the form:

$$\hat{U}(t,t_0) = \mathbb{1} + \sum_{n=1}^{\infty} (-i)^n \frac{1}{n!} \int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 \cdots \int_{t_0}^{t} dt_n \hat{T}\left(\hat{H}(t_1) \cdots \hat{H}(t_n)\right). \tag{9.14}$$

Note the presence of the corrective factor $\frac{1}{n!}$ due to the fact that the integral over each of the $n!$ possible combinations of the positions of t_i remains the same because the operator $\hat{T}$ always rearranges the t_i in such a way that they return to their initial positions. It is customary to condense the expression 9.14 into the form:

$$\hat{U}(t,t_0) = \hat{T}\left(e^{-i\int_{t_0}^{t} dt_1 \hat{H}(t_1)}\right). \tag{9.15}$$

Note 9.1.1. 1. If the Hamiltonian $\hat{H}$ is independent of time, then clearly $[\hat{H}(t_i), \hat{H}(t_j)] = 0$ for all t_i, t_j. As such, the operator $\hat{T}$ acts trivially on the product of Hamiltonians. So we have:

$$\begin{aligned}\hat{U}(t,t_0) &= \mathbb{1} + \sum_{n=1}^{\infty} (-i)^n \frac{1}{n!} \int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 \cdots \int_{t_0}^{t} dt_n \hat{T}\left(\hat{H}(t_1) \cdots \hat{H}(t_n)\right) \\ &= \mathbb{1} + \sum_{n=1}^{\infty} (-i)^n \frac{1}{n!} \int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 \cdots \int_{t_0}^{t} dt_n \hat{H}(t_1) \cdots \hat{H}(t_n),\end{aligned}$$

which, in exponential notation, gives $\hat{U}(t,t_0) = e^{-i\int_{t_0}^{t} dt_1 \hat{H}(t_1)}$. Moreover, since $\hat{H}$ is independent of time, $\int_{t_0}^{t} dt' \hat{H}(t') = \hat{H}(t-t_0)$, and the time evolution operator can be rewritten as $\hat{U}(t,t_0) = \left(e^{-i\hat{H}(t-t_0)}\right)$. As such we indeed recover the standard expression for the evolution under a time independent Hamiltonian (Eq.(9.3)).

2. In general, there is no guarantee that $\hat{T}\left(e^{-i\int_{t_0}^{t} dt_1 \hat{H}(t_1)}\right) = e^{-i\int_{t_0}^{t} dt_1 \hat{H}(t_1)}$. Therefore, you have to go back to the uncompressed expression 9.14 for $\hat{U}$ and explicitly compute each term of the expansion before summing them. This is generally pretty painful unless you get lucky and a recurrence relation between all the terms is found. Therefore, we usually focus on situations where we can limit the expansion to a few terms.

3. In the context of quantum computing it is common to attempt to approximate $\hat{U}(t,t_0)$ by breaking the continuous time evolution down into discrete time steps and use:

$$\hat{U}(t,t_0) \approx \prod_j e^{-i\hat{H}(t_j)\delta t} := \hat{U}_{\text{disc}}(t,t_0)\,.$$

where $\delta t = t/m_t$ for some integer m_t. It can be shown that the resulting approximation is upper bounded by

$$\left\| \int_{t_0}^{t} ds \hat{H}(s) - \delta t \sum_{r=1}^{m_t} \hat{H}(t_0 + r\delta t) \right\|^2 \tag{9.16}$$

where $\|...\|$ is any matrix norm that is unitarily invariant. The key thing to understand about this approximation is that you are effectively breaking the continuous evolution of the Hamiltonian down into discrete time blocks and assuming that each block (approximately) commutes.

9.2 Interaction Representation

You are already familiar with the formalism of quantum mechanics from the Heisenberg and Schrödinger perspectives. In this section, we introduce a new representation called the *interaction representation.*

Let's begin with some reminders:

1. In the Schrödinger representation, it is the states $|\phi_S(t)\rangle$ that explicitly depend on time. The evolution is governed by the following equation:

$$i\frac{\partial}{\partial t} |\phi_S(t)\rangle = \hat{H}(t) |\phi_S(t)\rangle\,.$$

In this representation, observables are fixed operators, and any time dependence they have, if at all, is intrinsic and not governed by $\hat{H}$.

Figure 9.2: I had no idea what is meant to be going on in this meme when I first saw it and just thought it would just make this page a little more colourful. Then someone sent me this link and I realised it was a brilliant explaination of the interaction picture. Credit: L'heure est grave.

2. In the Heisenberg viewpoint, the time dependence is instead transferred to the operators. The state vectors are assumed to be fixed, and their time dependence is intrinsic. The system's time evolution is governed by:

$$\begin{cases} |\phi_H(t)\rangle = |\phi_S(t_0)\rangle, \\ \hat{O}_H(t) = \hat{U}_S^\dagger(t,t_0)\hat{O}_S(t)\hat{U}_S(t,t_0) \end{cases}$$

3. These two definitions lead to identical expectation values:

$$\begin{aligned} \left\langle \phi_H(t) \middle| \hat{O}_H(t) \middle| \phi_H(t) \right\rangle &= \left\langle \phi_H(t) \middle| \hat{U}_S^\dagger(t,t_0)\hat{O}_S(t)\hat{U}_S(t,t_0) \middle| \phi_H(t) \right\rangle \\ &= \left\langle \hat{U}_S^\dagger(t,t_0)\phi_S(t) \middle| \hat{U}_S^\dagger(t,t_0)\hat{O}_S(t)\hat{U}_S(t,t_0) \middle| \hat{U}_S^\dagger(t,t_0)\phi_S(t) \right\rangle \\ &= \left\langle \hat{U}_S(t,t_0)\hat{U}_S^\dagger(t,t_0)\phi_S(t) \middle| \hat{O}_S(t) \middle| \hat{U}_S(t,t_0)\hat{U}_S^\dagger(t,t_0)\phi_S(t) \right\rangle \\ &= \left\langle \phi_S(t) \middle| \hat{O}_S(t) \middle| \phi_S(t) \right\rangle. \end{aligned}$$

In other words, both representations lead to the same physics and we are free to pick which ever one makes our calculations easiest.

The interaction representation is a kind of "blend" of these two points of view. We start with a problem described by a Hamiltonian of the form:

$$\hat{H}(t) = \hat{H}_0 + \hat{V}(t).$$

We will treat the time dependence due to the perturbation $\hat{V}$ as evolving the states (Schrodinger-style) and the time dependence due to $\hat{H}_0$ as evolving the observables (Heisenberg-style).

Let us start by defining the evolution of states and operators in the interaction picture as:

$$\begin{cases} \hat{O}_I(t) = e^{i\hat{H}_0(t-t_0)}\hat{O}_S(t)e^{-i\hat{H}_0(t-t_0)}, \\ |\phi_I(t)\rangle = e^{i\hat{H}_0(t-t_0)}|\phi_S(t)\rangle = e^{i\hat{H}_0(t-t_0)}\hat{U}_S(t,t_0)|\phi_S(t_0)\rangle. \end{cases} \tag{9.17}$$

It is straightforward to check that this is consistent with the Schrodinger picture as:

$$\begin{aligned}\left\langle \phi_I(t)\right| \hat{O}_I(t) \left|\phi_I(t)\right\rangle &= \langle \phi_S(t)| \, e^{-i\hat{H}_0(t-t_0)} e^{i\hat{H}_0(t-t_0)} \hat{O}_S(t) e^{-i\hat{H}_0(t-t_0)} e^{i\hat{H}_0(t-t_0)} \, |\phi_S(t)\rangle \\ &= \left\langle \phi_S(t)\right| \hat{O}_S(t) \left|\phi_S(t)\right\rangle .\end{aligned} \tag{9.18}$$

If this seems a little arbitrary and pointless currently, don't worry, it will hopefully become clearer in a bit while it is useful. But before we get there let's keep going with seeing how this representation works.

We can implicitly define the interaction evolution operator $\hat{U}_I(t,t_0)$ as:

$$|\phi_I(t)\rangle = \hat{U}_I(t,t_0) \, |\phi_I(t_0)\rangle$$

This, combined with the second equation in (9.17), gives us an explicit expression for $\hat{U}_I(t,t_0)$:

$$\hat{U}_I(t,t_0) = e^{i\hat{H}_0(t-t_0)} \hat{U}_S(t,t_0). \tag{9.19}$$

Let's now have a look at how such an operator evolves. Differentiating it gives:

$$\begin{aligned}\frac{\partial}{\partial t}\hat{U}_I(t,t_0) &= e^{i\hat{H}_0(t-t_0)} i\hat{H}_0\hat{U}_S(t,t_0) - ie^{i\hat{H}_0(t-t_0)}\hat{H}(t)\hat{U}_S(t,t_0) \\ &= -ie^{i\hat{H}_0(t-t_0)}\left(\hat{H}(t) - \hat{H}_0\right)\hat{U}_S(t,t_0) \\ &= -ie^{i\hat{H}_0(t-t_0)}\hat{V}(t)\hat{U}_S(t,t_0) \\ &= -ie^{i\hat{H}_0(t-t_0)}\hat{V}(t)e^{-i\hat{H}_0(t-t_0)}e^{i\hat{H}_0(t-t_0)}\hat{U}_S(t,t_0) \\ &= -i\hat{V}_I(t)\hat{U}_I(t,t_0).\end{aligned}$$

where in the final line we use the definition of an operator in the interaction picture from Eq.(9.17). Thus we have that the analogue of the Schrodinger equation for the evolution operator in the interaction picture is given by:

$$i\frac{\partial}{\partial t}\hat{U}_I(t,t_0) = \hat{V}_I(t)\hat{U}_I(t,t_0). \tag{9.20}$$

The key thing to notice is that in the equation that governs the evolution of the evolution operator in the interaction picture, i.e., Eq. (9.20), it is the perturbation that plays the role of the Hamiltonian! That is, we have simplified the differential equation we need to solve to find the propagator by hiding $\hat{H}_0$. If we push the analogy a bit further, we can use similar reasoning as we used to find the propagator in the Schrodinger picture, to obtain an expansion of $\hat{U}_I(t,t_0)$:

$$\begin{aligned}\hat{U}_I(t,t_0) &= \mathbb{1} + \sum_{i=1}^{\infty}(-i)^n \int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 \cdots \int_{t_0}^{t} dt_n \left(\hat{V}_I(t_1)\cdots\hat{V}_I(t_{n-1})\right) \\ &= \mathbb{1} + \sum_{i=1}^{\infty}(-i)^n \frac{1}{n!}\int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 \cdots \int_{t_0}^{t} dt_n \hat{T}\left(\hat{V}_I(t_1)\cdots\hat{V}_I(t_n-1)\right),\end{aligned} \tag{9.21}$$

which, similarly to before, we can also put in a more condensed version:

$$\hat{U}_I(t,t_0) = \hat{T}\left(e^{-i\int_{t_0}^{t} dt'\hat{V}_I(t')}\right).$$

As mentioned earlier, such an expansion is only meaningful if it is possible to truncate the sum from a certain term onwards. This is feasible when $\hat{V}(t)$ is a small perturbation.

9.3 Transition Probabilities

Consider a system described by a Hamiltonian of the form

$$\hat{H}(t) = \hat{H}_0 + \hat{V}(t) \tag{9.22}$$

where

$$\hat{V} = \begin{cases} 0 \text{ if } t \leq t_0 \\ \hat{V}(t) \text{ if } t > t_0. \end{cases} \tag{9.23}$$

We will use $|n\rangle$ and E_n to denote the states and eigenvalues of the unperturbed Hamiltonian. Suppose the system is in the eigenstate $|i\rangle$ at $t = t_0$, so its temporal evolution is determined by:

$$|\phi_S(t)\rangle = U_S(t, t_0)\,|i\rangle = \sum_{n=0}^{\infty} c_n(t)\,|n\rangle\,,$$

where $\sum_{n=0}^{\infty}|c_n|^2 = 1$. Since the states $|n\rangle$ are orthonormal, projecting the state $|\phi_S\rangle$ onto the state $|n\rangle$ determines the coefficient c_n, and this holds for any $n \in \mathbb{N}$:

$$\begin{aligned} c_n(t) = \langle n|\phi_S(t)\rangle &= \langle n|\hat{U}_S(t, t_0)|i\rangle \\ &= \langle n|e^{-i\hat{H}_0(t-t_0)}\hat{U}_I(t, t_0)|\,|i\rangle\rangle \\ &= e^{-i\frac{E_n(t-t_0)}{\hbar}}\langle n|\hat{U}_I(t, t_0)|i\rangle\,. \end{aligned}$$

The amplitude $c_n(t)$ is simply the amplitude to find the system in eigenstate $|n\rangle$ given that it started in state $|i\rangle$. Thus the transition probability $P_{i\to n}$ from the initial state $|i\rangle$ to any eigenstate $|n\rangle$ of $\hat{H}_0$ is simply the mod-square of this:

$$P_{i\to n} = |\langle n|\phi_S(t)\rangle|^2 = |c_n(t)|^2 = \left|\langle n|\hat{U}_I(t, t_0)|i\rangle\right|^2.$$

Note that by assumption $\hat{V}(t) = 0$ for all $t \leq t_0$, so $|i\rangle$ is not only an eigenstate of $\hat{H}_0$ but also of $\hat{H}$ for $t \leq t_0$. Let's determine the expression of the transition probability at the first order in $\hat{V}$. Note that (from Eq. (9.21)) in the first order in V the propagator is of the form:

$$\hat{U}_I(t, t_0) = \mathbb{1} - i\int_{t_0}^{t} dt_1 \hat{V}_I(t_1),$$

and so (assuming $n \neq i$) we have

$$\begin{aligned} \langle n|\hat{U}_I(t, t_0)|i\rangle &= -i\int_0^t dt_1\,\langle n|\hat{V}_I(t, t_0)|i\rangle \\ &= -i\int_{t_0}^{t} dt_1\,\langle n|e^{i\hat{H}_0(t_1-t_0)}\hat{V}(t_1, t_0)e^{-i\hat{H}_0(t_1-t_0)}|i\rangle \\ &= -i\int_{t_0}^{t} dt_1 e^{-i(E_n-E_i)(t_1-t_0)}\langle n|\hat{V}(t, t_0)|i\rangle\,, \end{aligned}$$

and finally

$$P_{i\to n} = \left|-i\int_{t_0}^{t} dt_1 e^{-i(E_n-E_i)(t_1-t_0)}\langle n|\hat{V}(t_1, t_0)|i\rangle\right|^2. \tag{9.24}$$

This is the first-order time-dependent perturbation theory expression for the computation of a transition probability. Let's now evaluate it for some common cases of interest.

Turning on a constant perturbation. Let's consider the special case where the potential (once turned on) does not depend on time. That is, let's suppose that

$$\hat{V} = \begin{cases} 0 \text{ if } t \leq t_0 \\ \hat{V} \text{ if } t > t_0, \end{cases}$$

and 9.24 becomes:

$$\begin{aligned} P_{i\to n}(t) &= \left| \langle n|\hat{V}|i\rangle \int_{t_0}^{t} dt_1 e^{-i(E_n - E_i)(t_1 - t_0)} \right|^2 \\ &= \left| \frac{1}{i} \langle n|\hat{V}|i\rangle \frac{e^{-i(E_n-E_i)(t-t_0)} - 1}{E_n - E_i} \right|^2 \\ &= \left|\langle n|\hat{V}|i\rangle\right|^2 \frac{4}{(E_n - E_i)^2} \sin^2\left(\frac{(E_n - E_i)(t - t_0)}{2}\right). \end{aligned}$$

Without loss of generality we can take $t_0 = 0$ and rewrite our expression for $P_{i\to n}(t)$ as

$$P_{i\to n}(t) = \left|\langle n|\hat{V}|i\rangle\right|^2 f\left(E_n - E_i\right), \tag{9.25}$$

with $f(\omega) = \frac{4}{\omega^2}\sin\left(\frac{\omega t}{2}\right)$ and $\omega = E_n - E_i$. The function $f(\omega)$ is sketched in Fig. 9.3. Note that:

$$f(\omega) = \begin{cases} 0 \text{ for } \frac{\omega t}{2} = k\pi \\ \\ \frac{4}{\omega^2} \text{ if } \frac{\omega t}{2} = \frac{\pi}{2} + k\pi, \end{cases}$$

where k is an integer. Thus we see that at a fixed time t, the probability of transitioning to a state $|n\rangle$ will be highest for those such that $\omega = E_n - E_i$ satisfies $\omega \leq \frac{2\pi}{t}$.

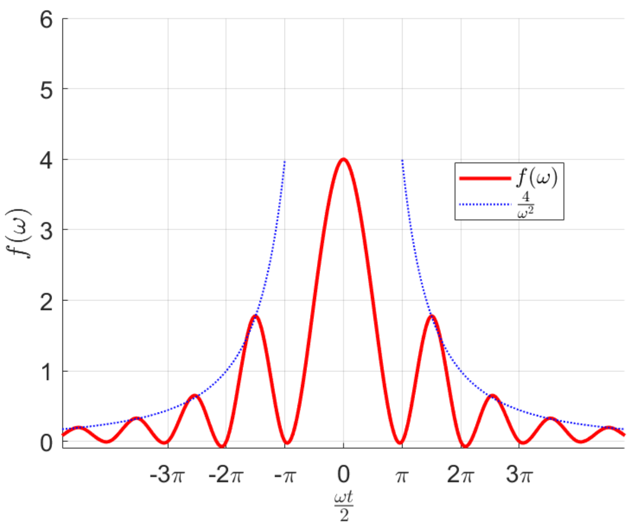


Figure 9.3: This is a plot of $f(\omega)$ where the horizontal axis is given in units of $\omega t/2$.

We now do something which is standard in physics textbook derivations but would make a mathematician cry [2] and say

$$\lim_{t\to\infty} \frac{\sin^2(xt)}{x^2} = \pi t \delta(x). \tag{9.26}$$

[2] I'm honestly all for 'physicist maths' normally but this one is a stretch even by my standards. If I find time I'll try and dig out a reference to a better derivation and/or write up one myself. If you come across one you like in the meantime feel free to email me. The discussion here might also make you feel a bit better.

We thus obtain the *Fermi golden rule*:

$$\lim_{t\to\infty} P_{i\to n}(t) = 4\left|\langle n|\hat{V}|i\rangle\right|^2 \lim_{t\to\infty}\frac{1}{\omega^2}\sin^2\left(\frac{\omega t}{2}\right) = 2\pi t\left|\langle n|\hat{V}|i\rangle\right|^2 \delta(E_n - E_i) \tag{9.27}$$

where the final line we use $\omega = E_n - E_i$.

It is sometimes more useful to work with a *transition probability per unit time*, in this case we have

$$\frac{\partial P_{i\to n}(t)}{\partial t} = 2\pi\left|\langle n|\hat{V}|i\rangle\right|^2 \delta(E_n - E_i)\,. \tag{9.28}$$

Oscillatory potential. Let's suppose now that the potential is given by

$$\hat{V} = \begin{cases} 0 \text{ if } t \le t_0 \\ \hat{V}(t)e^{i\omega t} + \hat{V}^\dagger e^{-i\omega t} \text{ if } t > t_0. \end{cases} \tag{9.29}$$

From Eq.(9.24), the equation for the transition probability is now given by:

$$\begin{aligned} P_{i\to n} &= \left|-i\int_0^t dt_1 e^{i(E_n-E_i)t_1}\left(\langle n|\hat{V}|i\rangle\, e^{i\omega t_1} + \langle n|\hat{V}^\dagger|i\rangle\, e^{-i\omega t_1}\right)\right|^2 \\ &= \left|\frac{1-e^{-i((E_n-E_i)+\omega)t}}{E_n - E_i + \omega}\langle n|\hat{V}|i\rangle + \frac{1-e^{-i((E_n-E_i)-\omega)t}}{E_n - E_i - \omega}\langle n|\hat{V}^\dagger|i\rangle\right|^2 . \end{aligned}$$

At long times, transitions to energy states with $E_n = E_i \pm \omega$ are favoured, and (via a similar analysis to above) we find:

$$\omega_{i\to n}(t) = 2\pi\left|\langle n|\hat{V}|i\rangle\right|^2 \delta(E_n - E_i + \omega) + 2\pi\left|\langle n|\hat{V}^\dagger|i\rangle\right|^2 \delta(E_n - E_i - \omega).$$

Notice that the first term in the sum corresponds to an energy loss by the system, while the second term represents an energy gain by the system. This variant of Fermi's golden rule is very important, as it explains how optical transitions occur in the presence of an oscillating external electromagnetic field, for instance, between levels of an atom or a solid due to application of laser light.

Nearly constant perturbation. Let's now consider the case of a nearly constant perturbation

$$\hat{V}(t) = \hat{V}e^{\epsilon t}$$

where ϵ is real and positive. Instead of turning on the perturbation at time t_0, we here assume that it turns on very slowly from $t = -\infty$. We will take the limit $\epsilon \to 0$ at the end of the calculation to describe a constant perturbation.

Let's write the perturbative expansion of $\hat{U}_I(t, -\infty)$. For the sake of simplicity, which will become clear later, we will use the first form for the propagator obtained before the introduction of the time-ordered operator (i.e. Eq. (9.6) but with $\hat{H} \to \hat{V}_I$):

$$\hat{U}_I(t, -\infty) = \hat{I} - i\int_{-\infty}^{t} dt_1 \hat{V}_I(t_1) - \int_{-\infty}^{t} dt_1 \int_{-\infty}^{t_1} dt_2 \hat{V}_I(t_1)\hat{V}_I(t_2) + \cdots. \tag{9.30}$$

Let's now look at the transition amplitude:

$$c_n(t) = e^{-iE_n t}\langle n|\hat{U}_I(t, t_0)|i\rangle \tag{9.31}$$

where we have omitted the constant phase $e^{iE_n t_0}$. Combining the previous two equations and now keeping terms to *second order* in $\hat{V}_I$ gives:

$$e^{iE_n t} c_n(t) = \underbrace{-i\int_{-\infty}^{t} dt_1 \langle n|\hat{V}_I(t_1)|i\rangle}_{I_1} \underbrace{- \int_{-\infty}^{t} dt_1 \int_{-\infty}^{t_1} dt_2 \langle n|\hat{V}_I(t_1)\hat{V}_I(t_2)|i\rangle}_{I_2}$$

Let's start with the first integral. The calculation here proceeds in the same manner as for a constant and oscillatory perturbations. First we recall that

$$\begin{aligned} \hat{V}_I(t) &= e^{i\hat{H}_0 t}\hat{V}(t)e^{-i\hat{H}_0 t\hbar} \\ &= e^{i\hat{H}_0 t}\hat{V}e^{\epsilon t}e^{-i\hat{H}_0 t\hbar} \end{aligned}$$

Using the properties of the eigenstate we then have:

$$\begin{aligned} I_1 &= \int_{-\infty}^{t} dt_1 \langle n|\hat{V}_I(t_1)|i\rangle = \langle n|\hat{V}|i\rangle \int_{-\infty}^{t} dt_1 e^{i[(E_n - E_i)t_1 - i\epsilon t_1]} \\ &= \langle n|\hat{V}|i\rangle \left. \frac{\exp\left(i((E_n - E_i)t_1 - i\epsilon t_1)\right)}{i(E_n - E_i - i\epsilon)} \right|_{-\infty}^{t} \end{aligned}$$

If we were to stop at the first order, we would find the golden rule as follows:

$$P_{i\to n} = |c_n(t)|^2 = |\langle n|\hat{V}|i\rangle|^2 \frac{e^{2\epsilon t}}{(E_n - E_i)^2 + \epsilon^2}$$

and so

$$\omega_{i\to n} = \frac{dP_{i\to n}}{dt} = |\langle n|\hat{V}|i\rangle|^2 \frac{2\epsilon e^{2\epsilon t}}{(E_n - E_i)^2 + \epsilon^2} \tag{9.32}$$

Let's check that our result here agrees with that obtained for the constant perturbation in the limit that $\epsilon \to 0$. To do so we first note that

$$\lim_{\epsilon\to 0} \frac{2\epsilon e^{2\epsilon t}}{x^2 + \epsilon^2} = 2\pi\delta(x)$$

and thus

$$\lim_{\epsilon\to 0} \frac{dP_{i\to n}}{dt} = 2\pi|\langle n|\hat{V}|i\rangle|^2 \delta\left(E_n - E_i\right). \tag{9.33}$$

That is, we find we do indeed regain the previous result in Eq. (9.28).

But what about to second order? Let's now calculate I_2:

$$I_2 = \int_{-\infty}^{t} dt_1 \int_{-\infty}^{t_1} dt_2 \sum_m \langle n|\hat{V}_I(t_1)|m\rangle \langle m|\hat{V}_I(t_2)|i\rangle$$

where we have introduced $\hat{I}$ as $\sum_m |m\rangle\langle m|$

$$\begin{aligned}
I_2 &= \sum_m \langle n|\hat{V}|m\rangle \langle m|\hat{V}|i\rangle \int_{-\infty}^{t} dt_1 \int_{-\infty}^{t_1} dt_2 \exp\left(i(E_n - E_m - i\epsilon)t_1\right) \exp\left(i(E_m - E_i - i\epsilon)t_2\right) \\
&= \sum_m \langle n|\hat{V}|m\rangle \langle m|\hat{V}|i\rangle \int_{-\infty}^{t} dt_1 \exp\left(i(E_n - E_m - i\epsilon)t_1\right) \left.\frac{\exp\left(i(E_m - E_i - i\epsilon)t_2\right)}{i(E_m - E_i - i\epsilon)}\right|_{-\infty}^{t_1} \\
&= \sum_m \langle n|\hat{V}|m\rangle \langle m|\hat{V}|i\rangle \int_{-\infty}^{t} dt_1 \exp\left(i(E_n - E_m - i\epsilon)t_1\right) \frac{\exp\left(i(E_m - E_i - i\epsilon)t_1\right)}{i(E_m - E_i - i\epsilon)} \\
&= -\sum_m \frac{\langle n|\hat{V}|m\rangle \langle m|\hat{V}|i\rangle \exp\left(i(E_n - E_i - 2i\epsilon)t\right)}{(E_m - E_i - i\epsilon)(E_n - E_i - 2i\epsilon)}
\end{aligned}$$

The term $\exp\left(i(E_n - E_i - 2i\epsilon)t\right)/(E_n - E_i - 2i\epsilon)$ is the same as in I_1 (except for $\epsilon \to 2\epsilon$, which doesn't change anything in the limit $\epsilon \to 0$). If we start from

$$\exp\left(iE_n t\right) c_n(t) = \hat{I} - i \int_{-\infty}^{t} dt_1 \hat{V}_I(t_1) - 1 \int_{-\infty}^{t} dt_1 \int_{-\infty}^{t_1} dt_2 \hat{V}_I(t_1)\hat{V}_I(t_2)$$

and replace the two previous results, we have

$$\begin{aligned}
P_{i\to n} = |c_t(t)|^2 &= \left| i \int_{-\infty}^{t} dt_1 \hat{V}_I(t_1) + 1 \int_{-\infty}^{t} dt_1 \int_{-\infty}^{t_1} \hat{V}_I(t_1)\hat{V}_I(t_2) \right|^2 \\
&= \left| \langle n|\hat{V}|i\rangle + \sum_m \frac{\langle n|\hat{V}|m\rangle \langle m|\hat{V}|i\rangle}{E_m - E_i - i\epsilon} \right|^2 \frac{e^{2\epsilon t}}{(E_n - E_i)^2 + \epsilon^2}
\end{aligned}$$

and

$$\lim_{\epsilon\to 0} \frac{dP_{i\to n}}{dt} = \omega_{i\to n} = 2\pi \left| \langle n|\hat{V}|i\rangle + \sum_m \frac{\langle n|\hat{V}|m\rangle \langle m|\hat{V}|i\rangle}{E_m - E_i - i0^+} \right|^2 \delta(E_n - E_i)$$

which is the second-order transition rate for a time-independent perturbation $\hat{V}$. Note the sum over intermediate states $|m\rangle$ typical of second-order perturbation. Here, a very suggestive image is that the system undergoes "virtual" transitions to states $|m\rangle$ without conserving energy since they occur in an arbitrarily short time before going to state $|n\rangle$.

Chapter 10

Variational Principle

10.1 General Idea:

Consider a physical system described by a Hamiltonian $\hat{H}$. Let's write H in terms of its eigen-decomposition $H = \sum_i E_i |\phi_i\rangle\langle\phi_i|$ where we suppose that the energy levels are labelled in increasing order with $E_i \le E_{i+1}$ with E_0 the ground state energy. It follows that for any state $|\psi\rangle$, the average energy of that state $\langle\psi|H|\psi\rangle$, will always be greater than or equal to the ground state energy E_0. This rather obvious[1] statement is given the name of the *variational principle*:

$$\langle\psi|H|\psi\rangle \ge E_0.$$

This inequality becomes an quality (again obviously) if and only if $|\psi\rangle = |\phi_0\rangle$, and ϕ_0 is non-degenerate. I think this statement hardly needs proving but in case its helpful here is that proof in the discrete case (and the continuous case easily follows by using properties of the integral):

$$\begin{aligned}
\langle\psi|\hat{H}|\psi\rangle &= \sum_{n=0}^{\infty} E_n \left|\langle\psi|\phi_n\rangle\right|^2 \\
&\ge E_0 \sum_{n=0}^{\infty} \left|\langle\psi|\phi_n\rangle\right|^2 \\
&= E_0 \sum_{n=0}^{\infty} \langle\psi|\phi_n\rangle\langle\phi_n|\psi\rangle \\
&= E_0
\end{aligned}$$

Note that I have provided the statement above assuming, as is standard, that the state $|\psi\rangle$ is normalised. However, the variational principle is often stated more generally for the case of a (potentially) non-normalized state. In this case you first need to normalize by hand such that $|\psi\rangle$ becomes $\frac{1}{\sqrt{\langle\psi|\psi\rangle}}|\psi\rangle$ and so the variational principle becomes:

$$\frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} \ge E_0\,. \tag{10.1}$$

We can use the variational principle to find an approximation of the ground state of H. The idea is to come up with a parameterised guess for the state $|\psi\rangle$, and then we use the variational

[1]I generally try and avoid calling things 'trivial' or 'obvious' but I really do think this statement is. And recognising so is actually helpful. Of course the lowest energy a state can have is the ground state energy! As a result I've always found naming this claim as the 'variational principle' at best a bit grandiose and at worst slightly confusing.

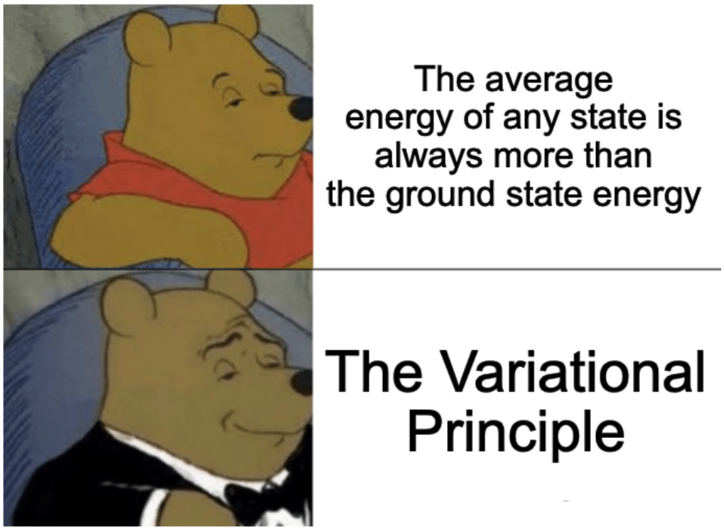


Figure 10.1:

principle to find the parameter values that minimize ψ. This method generalizes to excited states. For any $|\psi\rangle \in \mathcal{H}$ such that $\langle\phi_0|\psi\rangle = 0$, the following inequality[2] is always satisfied:

$$\frac{\langle\psi|\hat{H}|\psi\rangle}{\langle\psi|\psi\rangle} \geq E_1.$$

The proof of this fact is identical to the proof of the variational principle for the ground state since the term involving $|\phi_0\rangle$ drops out by the choice of $|\psi\rangle$.

Ok, so the basic idea of the variational principle is pretty simple (I promise!). Let's now look at how it is applied in practise. Again, I hope you'll agree that the basic idea of how to apply it is straightforward enough. That said, as we'll see, actually doing the full calculation can lead to some annoying integrals.

Example 10.1.1 (One-Dimensional Harmonic Oscillator). The system's Hamiltonian is given by:

$$\hat{H} = \underbrace{-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}}_{=\hat{T}} + \underbrace{\frac{1}{2}m\omega^2 x^2}_{=\hat{V}}. \tag{10.2}$$

We introduce a (non-normalized) trial function:

$$\psi_a(x) = \frac{1}{x^2 + a} \tag{10.3}$$

with $a > 0$. Note that this choice is physically unrealistic because the wavefunction should decrease exponentially as x goes to infinity. Our goal is to compute the energy of H in the state

[2]We're assuming here that the ground state is non-degenerate. If it's degenerate you need the constraint that $|\psi\rangle$ has zero overlap onto the space spanned by the ground states.

$|\psi\rangle$ and then find the a that minimizes this energy. To do so, we need to compute:

$$\begin{aligned}\langle\psi|\hat{T}|\psi\rangle &= -\frac{\hbar^2}{2m}\int_{-\infty}^{\infty} dx \frac{1}{x^2+a}\frac{d^2}{dx^2}\frac{1}{x^2+a}\\ \langle\psi|\hat{V}|\psi\rangle &= \frac{1}{2}m\omega^2\int_{-\infty}^{\infty} dx\frac{x^2}{(x^2+a)^2}\\ \langle\psi|\psi\rangle &= \int_{-\infty}^{\infty} dx\frac{1}{(x^2+a)^2}\,.\end{aligned} \tag{10.4}$$

This will allow us to compute the average energy of our guess as a function of x as

$$E(x) := \frac{\langle\psi|\hat{H}|\psi\rangle}{\langle\psi|\psi\rangle} = \frac{\langle\psi|\hat{T}|\psi\rangle}{\langle\psi|\psi\rangle} + \frac{\langle\psi|\hat{V}|\psi\rangle}{\langle\psi|\psi\rangle}\,. \tag{10.5}$$

And then all we need to do is find the minimum of the function $E(x)$, and this will be our guess of the ground state energy.

Computing the integrals is the hard part. I'll leave that fun to you and just state the results here [3].

$$\langle\psi|\psi\rangle = \int_{-\infty}^{\infty}\frac{1}{(x^2+a)^2}dx = \frac{\pi}{2a^{3/2}} \tag{10.6}$$

$$\begin{aligned}\langle\psi|\hat{H}|\psi\rangle &= \int_{-\infty}^{\infty}\frac{1}{x^2+a}\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+\frac{1}{2}m\omega^2x^2\right)\frac{1}{x^2+a}dx\\ &= -\frac{\hbar^2}{2m}\int_{-\infty}^{\infty}\frac{6x^2-2a}{(x^2+a)^4}dx + \frac{1}{2}m\omega^2\int_{-\infty}^{\infty}\frac{x^2}{(x^2+a)^2}dx\\ &= \frac{\pi}{2a^{3/2}}\left(\frac{\hbar^2}{4ma}+\frac{1}{2}m\omega^2 a\right)\,.\end{aligned} \tag{10.7}$$

The energy corresponding to a state $|\psi_a\rangle$ is therefore given by

$$E(a) = \frac{\langle\psi_a|\hat{H}|\psi_a\rangle}{\langle\psi_a|\psi_a\rangle} = \frac{\hbar^2}{4m}\frac{1}{a}+\frac{1}{2}m\omega^2 a,$$

and we seek a such that the energy is minimal:

$$\frac{dE(a)}{da} = -\frac{\hbar^2}{4ma^2}+\frac{1}{2}m\omega^2 = 0 \implies \frac{1}{2}m\omega^2a^2 = \frac{\hbar^2}{4m} \implies a = \frac{\hbar}{m\omega\sqrt{2}}.$$

Our approximation of the energy of the ground state is therefore given by

$$E\left(\frac{\hbar}{m\omega\sqrt{2}}\right) = \frac{\hbar\omega}{\sqrt{2}} \simeq 0.72\hbar\omega \tag{10.8}$$

This approximation is considerably higher than the exact (known in the case of the harmonic oscillator) ground state energy: $0.72\hbar\omega > 0.5\hbar\omega$.

[3] Don't worry, in the exam I'll give you enough hints for you to be able to figure it out without being an integration wizard. If you want some hints for this one, go check out Vincenzo's notes.

Example 10.1.2 (One-Dimensional Harmonic Oscillator:). We could now similarly determine the first excited state of the one-dimensional harmonic oscillator. The Hamiltonian is still given by Eq. 10.2. Let's set [4] $\psi_a(x))\frac{x}{(x^2+a)^2}$ with $a > 0$. This function is odd under the inversion $x \to -x$. Therefore, it will be orthogonal to the ground state $\psi_0(x)$, which is even.

For the computation, we will need the following integrals:

$$I_4 = \int_{-\infty}^{\infty} dx \frac{1}{(x^2+a)^4} = \frac{5\pi}{16} a^{-7/2} \qquad I_5 = \frac{35\pi}{128} a^{-9/2}$$

$$J_4 = \int_{-\infty}^{\infty} \frac{x^2}{(x^2+a)^4} = \frac{\pi}{16} a^{-5/2} \qquad I_6 = \frac{63\pi}{256} a^{-11/2}$$

$$k_4 = \int_{-\infty}^{\infty} dx \frac{x^4}{(x^2+a)^4} = \frac{\pi}{16} a^{-3/2}$$

It follows that we can compute the kinetic energy term as:

$$\begin{aligned}
\langle \phi_a | \hat{T} | \phi_a \rangle &= -\frac{\hbar^2}{2m} \int_{-\infty}^{\infty} dx \frac{x^2}{(x^2+a)^2} \frac{d^2}{dx^2} \frac{x^2}{(x^2+a)^2} = \cdots \\
&= \frac{\hbar^2}{2m} \int_{-\infty}^{\infty} dx \left(\frac{d}{dx} \frac{x}{(x^2+a)^2} \right)^2 \\
&= \frac{\hbar^2}{2m} \int_{-\infty}^{\infty} dx \left(-\frac{1}{(x^2+a)^2} - \frac{4x^2}{(x^2+a)^3} \right)^2 \\
&= \frac{\hbar^2}{2m} \int_{-\infty}^{\infty} dx \left(-\frac{3}{(x^2+a)^2} + \frac{4a}{(x^2+a)^3} \right)^2 \\
&= \frac{\hbar^2}{2m} \left(9I_4 - 24aI_5 + 16a^2 I_6 \right) \\
&= \frac{\hbar^2}{2m} \left(\frac{45\pi}{16} - \frac{105\pi}{16} + \frac{63\pi}{16} \right) a^{-7/2} \\
&= \frac{3}{16} \pi \frac{\hbar^2}{2m} a^{-7/2}
\end{aligned}$$

And the potential energy term is given by:

$$\begin{aligned}
\langle \phi_a | \hat{V} | \phi_a \rangle &= \frac{1}{2} m\omega^2 \int_{-\infty}^{\infty} dx \frac{x^4}{(x^2+a)^4} \\
&= \frac{1}{2} m\omega^2 k_4 \\
&= \frac{\pi}{32} m\omega^2 a^{-3/2}
\end{aligned}$$

Finally, the norm is given by:

$$\langle \phi_a | \phi_a \rangle = \int_{-\infty}^{\infty} dx \frac{x^2}{(x^2+a)^2} = J_4 = \frac{\pi}{16} a^{-5/2}$$

[4]Note we chose to divide by $(x^2+a)^2$ rather than (x^2+a^2). This is because if we picked $x/(x^2+a^2)$ then even those the function is square-integrable the potential term would eventually diverge.

Thus putting this mess together we have

$$E(a) = \frac{1}{2}\left(\frac{3\hbar^2}{m}a^{-7/2} + m\omega^2 a^{-3/2}\right)\cdot\left(a^{-5/2}\right)^{-1} = 3\frac{\hbar^2}{2m}\frac{1}{a} + \frac{1}{2}m\omega^2 a \tag{10.9}$$

To find our approximation of the energy of the first excited state we just minimize this:

$$\begin{aligned}
\frac{dE(a)}{da} &= -3\frac{\hbar^2}{2m}\frac{1}{a^2} + \frac{1}{2}m\omega^2 \\
\frac{dE(a)}{da} &= \Rightarrow \frac{3\hbar^2}{2m}\frac{1}{a^2} = \frac{1}{2}m\omega^2 \\
\Rightarrow a^2 &= \frac{3\hbar^2}{m^2\omega^2} \\
a = &= \sqrt{3}\frac{\hbar}{m\omega} \\
E_1(a) &= \frac{3\hbar^2}{2m}\frac{m\omega}{\hbar\sqrt{3}} + \frac{\sqrt{3}}{2}\hbar\omega
\end{aligned} \tag{10.10}$$

Thus we approximate the energy of the first excited state as:

$$E_1(a) = \sqrt{3}\hbar\omega \simeq 1.732\hbar\omega,$$

which is larger than, but not too far off, the known of the energy of the first excited state of the oscillator of $E_1^{\text{eff}} = 1.5\hbar\omega$.

More generally, if one cannot use a symmetry argument, one can always seek a state $|\phi\rangle$ that minimizes the energy expectation value, $E = \langle\phi|\hat{H}|\phi\rangle / \langle\phi|\phi\rangle$ with the constraint $\langle\phi|\psi\rangle = 0$, where $|\psi\rangle$ is the variational solution found for the ground state. If $|\psi\rangle$ is a good approximation, then its component orthogonal to $|0\rangle$ will be minimal. In this case, there is a high probability that the variational solution $|\phi\rangle$ will be almost orthogonal to $|0\rangle$ and will also provide a relatively good approximation to $|1\rangle$.

Note 10.1.3. Note that the variational approach makes error calculations extremely complicated (we can't do it unless we have a better approximation - but then we would just use that in the first place!) Furthermore, for any arbitrary wave function ψ, minimizing the error actually leads to restoring the Schrödinger equation.

10.2 The variational Principle for an arbitrary ansatz

These final two sections are non-examinable. I include them in case you are interested.

We can try to find the exact solution to the problem using the variational approach. Consider a Hamiltonian $\hat{H}$ and an arbitrary state $\psi(x)$. The energy expectation value is given by

$$E[\psi,\psi^*] = \langle\psi|\hat{H}|\psi\rangle = \int dx\psi^*\hat{H}\psi$$

Since ψ is a complex-valued function, we consider E to be a function of ψ and ψ^* (i.e., of $\Re(\psi)$ and $\Im(\psi)$).

Introduce an infinitesimal variation $\delta\psi^*(x)$ of $\psi^*(x)$, with $\delta\psi^*(x)\to 0$. We are treating ψ and ψ^* as two independent variables, and thus

$$E[\psi,\psi^*+\delta\psi^*] = \int dx\psi^*\hat{H}\psi + \int dx\delta\psi^*\hat{H}\psi$$

and

$$\delta E = E[\psi,\psi^*+\delta\psi^*] - E[\psi,\psi^*] = \int dx\delta\psi^*\hat{H}\psi$$

It is necessary to introduce the concept of a functional derivative at this point. Alternatively, we can imagine a function ψ "discretized" on a grid x_j, $j=-\infty,\cdots,1,2,\cdots$. In this case, we can interpret this problem in a variational context with an infinite number of parameters $\delta\psi_j^* = \delta^*(x_j)$. This way, we recover the concept of a traditional derivative.

To minimize E, we need $\delta E = 0$. Now,

$$\delta E = \int dx\delta\psi^*\hat{H}\psi$$

In the discretized version,

$$\delta E = \sum_j \delta\psi_j^*\hat{H}\psi_j$$

and the (true) derivative of E with respect to ψ_j^* is

$$\frac{\partial E}{\partial\psi_j^*} = \hat{H}\psi_j$$

The minimization condition is then

$$\frac{\partial E}{\partial\psi_j^*} = \ \forall j \Rightarrow \hat{H}\psi_j = 0\ \forall j \Rightarrow \psi_j = 0$$

and similarly for ψ_j^*.

This strange result is because we forgot the norm constraint. We need $\langle\psi|\psi\rangle = 1$. And if we do not have this, we can ways just set $\psi_j = 0$ to set the energy to 0.

To find a constrained minimum, we use the Lagrange multipliers. We want to minimize $\langle\psi|\hat{H}|\psi\rangle$ with the constraint $\langle\psi|\psi\rangle = 1$. We introduce the functional

$$E[\psi,\psi^*,\lambda] = \langle\psi|H|\psi\rangle - \lambda(\langle\psi|\psi\rangle - 1) = \int dx\psi^*\hat{H}\psi - \lambda\Big(\int dx\psi^*\psi - 1\Big)$$

As before:

$$\delta E = \int dx \delta\psi^* \hat{H}\psi - \lambda \int dx \delta\psi^* \psi$$

The condition $\delta E = 0$ for arbitrary variation $\delta\psi^*(x)$ implies equality of the integrands:

$$\hat{H}\psi = \lambda\psi$$

It's the Schrödinger equatioN! The variational principle, without additional conditions, should lead to the exact solution of the problem (but hasn't made the problem any easier).

Reminder 10.2.1. (Harmonic Oscillator[5]). We have

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2$$

with $[\hat{x}, \hat{p}] = i\hbar$. Let's introduce

$$\begin{aligned}
\hat{a} &\equiv \sqrt{\frac{m\omega}{2\hbar}}\hat{x} + i\frac{1}{\sqrt{2m\hbar\omega}}\hat{p} \\
\hat{a}^\dagger &\equiv \sqrt{\frac{m\omega}{2\hbar}}\hat{x} - i\frac{1}{\sqrt{2m\hbar\omega}}\hat{p} \\
\hat{x} &= \sqrt{\frac{\hbar}{2m\omega}}(\hat{a}^\dagger + \hat{a}) \\
\hat{p} &= i\sqrt{\frac{m\hbar\omega}{2}}(\hat{a}^\dagger - \hat{a})
\end{aligned}$$

We note

$$[\hat{a}, \hat{a}^\dagger] = \hat{a}\hat{a}^\dagger - \hat{a}^\dagger\hat{a} = 1$$

There is a ground state $|\phi_0\rangle$ such that

$$\hat{a}|\phi_0\rangle = 0$$

The spectrum is

$$\hat{H}|\phi_n\rangle = \hbar\omega\left(n + \frac{1}{2}\right)|\phi_n\rangle$$

The norms are

$$\begin{aligned}
\hat{a}^\dagger|\phi_n\rangle &= \sqrt{n+1}\,|\phi_{n+1}\rangle \\
\hat{a}|\phi_n\rangle &= \sqrt{n}\,|\phi_{n-1}\rangle \\
|\phi_n\rangle &= \frac{(\hat{a}^\dagger)^n}{\sqrt{N!}}|\phi_0\rangle
\end{aligned}$$

The $\{|\phi_n\rangle\}$ are non-degenerate, we thus have $\langle\phi_i|\phi_j\rangle = \delta_{ij}$.

Note 10.2.2.

$$\langle\phi_n|\hat{x}|\phi_n\rangle = \langle\phi_n|\hat{p}|\phi_n\rangle = 0$$

[5] Vincenzo Savona's notes, which I am working from here, have a couple of pages recapping the quantum harmonic osccilator at this point. It's not entirely clear to me why. So I will skip in the lecture. But Physicists love modelling things as a harmonic osccilator so it is good to have this stuff dialled so I'll this here in the notes in case it is helpful for anyone.

and

$$\langle\phi_n|\hat{x}^2|\phi_n\rangle = \cdots = \frac{\hbar}{2m\omega}(2n+1)$$
$$\langle\phi_n|\hat{p}^2|\phi_n\rangle = \cdots = \frac{m\hbar\omega}{2}(2n+1)$$

for $n = 0$ we have $\Delta\hat{x}\Delta\hat{p} = \frac{\hbar}{2}$

For a Harmonic oscillator in isotropic 3D, we have

$$\hat{H} = \frac{|\hat{\mathbf{p}}|^2}{2m} + \frac{1}{2}m\omega^2|\hat{\mathbf{r}}|^2$$

Note 10.2.3.

$$|\hat{\mathbf{p}}|^2 = \hat{p}_x^2 + \hat{p}_y^2 + \hat{p}_z^2$$
$$|\hat{\mathbf{x}}|^2 = \hat{x}^2 + \hat{y}^2 + \hat{z}^2$$

thus

$$\hat{H} = \hat{H}_x + \hat{H}_y + \hat{H}_z$$
$$\hat{H} = \frac{\hat{p}_x^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2$$
$$\hat{H} = \frac{\hat{p}_y^2}{2m} + \frac{1}{2}m\omega^2\hat{y}^2$$
$$\hat{H} = \frac{\hat{p}_z^2}{2m} + \frac{1}{2}m\omega^2\hat{z}^2$$

Separable hamiltonian:

$$\psi(x,y,z) = \psi_n(x)\phi_m(y)\xi_l(z)$$

where $\hat{H}_x\psi_n(x) = E_n\psi(x)$, with $E_n = \hbar\omega\left(n + \frac{1}{2}\right)$, similarly for $\hat{y}$ and $\hat{z}$. Thus $\hat{H}\psi = E_{nml}\psi$, with $E_{nml} = \hbar\omega\left(n + m + l + \frac{3}{2}\right)$ Why is the harmonic oscillator so important?

1. Except for pathological cases, all systems admit a harmonic approximation.

   Example 10.2.4. Central Potential. We have

   $$V = -\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial r^2} + \frac{L^2}{2mr^2} - \frac{\alpha}{r}$$

   One could start from the solution of the harmonic problem and calculate more accurate solutions using perturbation theory.

2. Quantum Field Theory for Multi-Body Systems. The state of a free particle with momentum $\hbar k$ corresponding to one quantum of energy can be written as $|1\rangle$. Thus, two particles in the same state will have twice the energy, which can be understood as the state $|2\rangle$ of the harmonic oscillator, and so on. The states of N free particles are described as an infinite set of harmonic oscillators, one for each $\hbar\mathbf{k}$.

   More formally, this result can be obtained from the consideration that the wave function $\psi(\mathbf{r})$ can be treated as a dynamic variable, and thus as an additional operator, denoted by $\hat{\psi}$ and $\hat{\psi}^\dagger$. This procedure is called second quantization.

10.3 Hartree-Fock Theory

Let's consider a system of N spinless Fermions. If you've forgotten the lecture of indistinguishable particles now might be a good moment to go back and revise it. But just to recap the basics, the state of such a system is anti-symmetric under exchange of any two particle indices. Thus we can write the general state as:

$$|\psi_{\mathbf{x}}\rangle = \frac{1}{\sqrt{N!}} \sum_{\mathbb{P} \in S_n} \text{sign}(\mathbb{P})\mathbb{P}|x_1, x_2, \ldots, , x_N\rangle \tag{10.11}$$

where $\text{sign}(\mathbb{P}) = -1$ if $\mathbb{P}$ involves an odd number of index swaps and $\text{sign}(\mathbb{P}) = 1$ if $\mathbb{P}$ involves an even number of index swaps. We note that given the Pauli exclusion principle, no two Fermions can be in the same state (i.e. $n_k = 1$ for all k), so each state in the sum here is unique and so the normalization is simply $\frac{1}{\sqrt{N!}}$.

Now, it'll be convenient here to switch notation and write this in terms of the wavefunctions explicitly. That is, we will work within the Hilbert space $\mathcal{H}_1$ of single-particle states, where the set $\{\phi_{n_i}\}_{i=1}^{N}$ represents an orthonormal basis of single-particle wave functions. Under these considerations, any wave function for N particles ψ can be expressed as:

$$\psi(x_1, \cdots, x_N) = \frac{1}{\sqrt{N!}} \sum_{\mathbb{P} \in S_n} \text{sign}(\mathbb{P})\mathbb{P}\phi_{n_1}(x_1) \quad \cdots \phi_{n_N}(x_N) \tag{10.12}$$

Or, equivalently, we can recognise this expression as a determinant and can write:

$$\psi(x_1, \cdots, x_N) = \frac{1}{N!} \begin{vmatrix} \phi_{n_1}(x_1) & \cdots & \phi_{n_N}(x_N) \\ \vdots & & \vdots \\ \phi_{n_N}(x_1) & \cdots & \phi_{n_N}(x_N) \end{vmatrix}. \tag{10.13}$$

We can now use our new found appreciation for the variational principle and can consider the ϕ_{n_i} as variational parameters. The Hartree-Fock approximation involves representing the ground state as a single Slater determinant, so we need to choose the ϕ_{n_i} that provide the best approximation.

The Hamiltonian of the system is given by $\hat{H} = \hat{T} + \hat{V}$, where

- The operator $\hat{T}$ is the total kinetic energy of the system, which is the sum of the kinetic energies of the N particles:
$$\hat{T} = \sum_{j=1}^{N} \hat{t}_j = \sum_{j=1}^{N} -\frac{\hbar}{2m}\nabla_j^2$$

- The operator $\hat{V}$ represents the potential energy of the N particles, given as the sum of potential energies of each pair of particles:
$$\hat{V} = \sum_{\substack{i,j \\ i \neq j}} \hat{V}_{i,j},$$
where $\hat{V}_{i,j} = \hat{V}(x_i, x_j)$.

We work within the Fock space. We have:

$$\langle\psi|\hat{T}|\psi\rangle = \sum_{j=1}^{N} \langle\phi_{n_j}|\hat{T}|\phi_{n_j}\rangle = \sum_{j=1}^{N} \int dx \phi_{n_j}^*(x) T(x) \phi_{n_j}(x), \tag{10.14}$$

and

$$\langle\psi|\hat{V}|\psi\rangle = \frac{1}{2}\sum_{i,j=1}^{N}\left(\langle\phi_{n_i}\phi_{n_j}|\hat{V}|\phi_{n_i}\phi_{n_j}\rangle - \langle\phi_{n_i}\phi_{n_j}|\hat{V}|\phi_{n_j}\phi_{n_i}\rangle\right) \tag{10.15}$$

$$= \frac{1}{2}\sum_{i,j=1}^{N}\int dx_1 dx_2\Bigg(\phi^*_{n_i}(x_1)\phi^*_{n_j}(x_2)\hat{V}(x_1,x_2)\phi_{n_i}(x_1)\phi_{n_j}(x_2) \tag{10.16}$$

$$- \phi^*_{n_j}(x_1)\phi^*_{n_i}(x_2)\hat{V}(x_1,x_2)\phi_{n_i}(x_1)\phi_{n_j}(x_2)\Bigg). \tag{10.17}$$

You should recognise this type of expression from when we studied indistinguishable particles - first term in the expression for $\langle\psi|\hat{V}|\psi\rangle$ is called the "direct term," while the second is the "exchange term."

The goal is to minimize $\langle\psi|\hat{H}|\psi\rangle = \langle\psi|\hat{T}|\psi\rangle + \langle\psi|\hat{V}|\psi\rangle$ subject to the N^2 constraints: $\langle\phi_{n_i}|\phi_{n_j}\rangle = \delta_{i,j}$. We use Lagrange multipliers to solve the constrained minimization problem.

Theorem 10.3.1 (Constrained Extrema via Lagrange multipliers)**.** *Seeking the extrema of a function $F(x,y)$ under a constraint $f(x,y) = 0$ is equivalent to searching for those of the function:*

$$H(x,y,\lambda) = F(x,y) - \lambda f(x,y).$$

Thus we are tasked with minimizing:

$$F = \langle\psi|\hat{H}|\psi\rangle - \sum_{i,j}\lambda_{i,j}\left(\langle\phi_{n_i}|\phi_{n_j}\rangle - \delta_{ij}\right). \tag{10.18}$$

We have N^2 constraints of the form $\langle\phi_{n_i}|\phi_{n_j}\rangle = \delta_{i,j}$ so initially it might seem that we need to introduce N^2 Lagrange multipliers. However, with a little thought we can see that the constraints with respect to swapping i and j and so it follows that $\lambda_{i,j} = \lambda^*_{i,j}$ which halves the number of constraints we need to deal with.

We consider ϕ and ϕ^* as independent variables. As an example, the variations with respect to $\phi^*_{n_i}$ yield:

$$\delta\hat{T} = \sum_j \int dx\delta\phi^*_{n_j}(x)\hat{t}\phi_{n_j}(x).$$

Similarly, the variations in $\hat{V}$ are:

$$\delta\hat{V} = \sum_{j\neq i}\int dx_1\int dx_2\Bigg(\delta\phi^*_{n_i}(x_1)\phi^*_{n_j}(x_2)\hat{V}\phi_{n_i}(x_1)\phi_{n_j}(x_2) - \delta\phi^*_{n_i}(x_2)\phi^*_{n_j}(x_1)\hat{V}\phi_{n_i}(x_1)\phi_{n_j}(x_2)\Bigg).$$

And the variations in the constraint term give:

$$\delta\sum_{i,j}\lambda_{i,j}\left(\langle\phi_{n_i}|\phi_{n_j}\rangle - 1\right) = \sum_{i,j}\lambda_{i,j}\int dx\delta\phi^*_i(x)\phi_j(x).$$

We want to minimize $F = \langle\psi|\hat{H}|\psi\rangle - \sum_{i,j}\lambda_{i,j}\left(\langle\phi_{n_i}|\phi_{n_j}\rangle - \delta_{ij}\right)$ with respect to ϕ_{n_i}. We, therefore, impose $\frac{\delta F}{\delta\phi^*_{n_i}} = 0$ for all i, which leads to the equation:

$$\hat{t}\phi_{n_i}(x) + \sum_{j=1}^{N}\int dx_2\Bigg(\phi^*_{n_j}(x_2)\hat{V}\phi_{n_i}(x)\phi_{n_j}(x_2) - \phi^*_{n_j}(x)\hat{V}\phi_{n_i}(x)\phi_{n_j}(x_2)\Bigg) = \sum_{j=1}^{N}\lambda_{i,j}\phi_{n_j}(x). \tag{10.19}$$

Without loss of generality we can chose to work in the basis in which the matrix λ is diagonal. That is, without loss of generality we can take $\lambda_{i,j} = \epsilon_i \delta_{i,j}$ and we end up with *the Hartree-Fock equation* :

$$-\frac{\hbar^2}{2m}\nabla^2\phi_{n_i}(x) + \sum_{j=1}^{N}\int dx_2\Big(\phi^*_{n_j}(x_2)\hat{V}\phi_{n_i}(x)\phi_{n_j}(x_2) - \phi^*_{n_j}(x)\hat{V}\phi_{n_i}(x)\phi_{n_j}(x_2)\Big) = \epsilon_i\phi_{n_i}(x). \tag{10.20}$$

Or, equivalently, we can write this more compactly as:

$$(T(x) + V_H(x) - V_E(x))\,\phi_{n_i}(x) = \epsilon_i\phi_{n_i}(x) \tag{10.21}$$

where we have defined

$$\begin{aligned} T(x) &:= -\frac{\hbar^2}{2m}\nabla^2 \\ V_H(x) &:= \sum_{j=1}^{N}\int dx_2\phi^*_{n_j}(x_2)\hat{V}\phi_{n_j}(x_2) \\ V_E(x) &:= \sum_{j=1}^{N}\int dx_2\phi^*_{n_j}(x)\hat{V}\phi_{n_j}(x_2)\,. \end{aligned} \tag{10.22}$$

Thus we see that we have decoupled the original eigenvalue problem defined on the N particle system into a set of N eigenvalue problems for each of the single particle states. This looks easier! The first term is the kinetic term, the second term is a potential energy term (which we will look at more closely in a second) and the third term is the 'exchange term' arising from the anti-symmetrization properties of the fermionic wave-function.

Ok, let us look more carefully at the $V_H(x)$ term (which corresponds to the direct integral term in the potential 10.17). Let's suppose that the potential has the form:

$$\hat{V}(x_1, x_2) = \frac{e^2}{|x_1 - x_2|} \tag{10.23}$$

We can then rewrite the Hartree term as:

$$\begin{aligned} \hat{V}_H(x) &= \sum_{j=1}^{N}\int dx_2 e^2\frac{\left|\phi_{n_j}(x_2)\right|^2}{|x - x_2|} \\ &= e^2\int dx_2\frac{\sum_{j=1}^{N}\left|\phi_{n_j}(x)\right|^2}{|x - x_2|} \\ &= e^2\int dx_2\frac{\rho(x_2)}{|x - x_2|},. \end{aligned}$$

That is, the second term in the Hartree Fock equation can be interpreted as an effective potential generated by the average potential generated by surrounding particles. That is, the *Hartree potential energy is a functional of the density* $\rho(x)$, as ρ is a function of a single variable. Note, however, that the potential term depends on the wave-functions of all the other electrons.

If the exchange term V_E is negligible, then the initial N-body problem reduces to a one-body problem leading to the simplified Hartree equation:

$$-\frac{\hbar^2}{2m}\nabla^2\phi_{n_i}(x) + \hat{V}_H(x)\phi_{n_i}(x) = \epsilon_i\phi_{n_i}(x). \tag{10.24}$$

The Hartree energy is then given by:

$$E = \sum_{i=1}^{N} \langle \phi_{n_i} | \hat{t} | \phi_{n_i} \rangle + \int dx_1 \int dx_2 e^2 \frac{\rho(x_1)\rho(x_2)}{|x_1 - x_2|}. \tag{10.25}$$

While the Hartree equation has simplified the problem in the sense that we now have a set of equations for each of the one-body wavefunctions, solving these exactly is challenging as the potential term depends on the wavefunctions of all the particles via the density term $\rho(x)$. So to go further the general strategy is to pick a clever guess functional form for the density and then apply the variational principle. This is the core idea of what is known as *density functional theory* - a very powerful and widely used tool for approximating the energetic structure of many-body systems. At its core is the following Theorem:

Theorem 10.3.2 (First Hohenberg-Kohn Theorem)**.** *The energy E of the ground state of an N-particle system defined by $\hat{H}$ is an unknown functional of the density $\rho(x)$.*

If you are interested in knowing more on this I recommend Giuseppe Carleo's master's course on methods for simulating quantum systems.

Let $|\psi_1\rangle, |\psi_2\rangle, |\psi_3\rangle \in \mathcal{H}_1$, $|\phi\rangle \in \mathcal{H}_2$, $\dim(\mathcal{H}_1) > \dim(\mathcal{H}_2)$

$\lvert\psi_1\rangle$	$\lvert\psi_1\rangle \lvert\phi\rangle$
$\lvert\psi_1\rangle \lvert\psi_2\rangle$	$\lvert\psi_1\rangle \langle\psi_3\rvert$

Table 1: Is this loss?

Figure 10.2: And let's end with one more meme. I originally gave this the wooden spoon award because my reaction, similarly to many of you I guess, was 'is this even a meme?'. But having now had it explained to me I have to concede its pretty clever. And if you don't get it - that's just a healthy sign that you don't spend too too much time online.

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