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# Semi-classical mechanics for interacting electrons

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## Introduction

Semi-classical mechanics is a subject in which we try to solve problems that are too complicated to solve using proper quantum mechanics. As the number of interacting particles increases, differential equations become more and more complicated. Putting the impossibility of finding analytical solutions to wave function for many-particle systems aside, even numerically it is a very time-consuming process to solve such systems. Semi-classical mechanics usually uses some ideas from classical formalisms, like phase space, Hamiltonian, action, etc., and use them to create a classical trajectory onto which quantum phenomena are imposed in different ways. Hence, good knowledge of each of these subfields is necessary to understand the modelings in Semi-classical mechanics. In the following sections, the theory of Semi-classical mechanics is developed in pieces. Starting with the basics of linear algebra and quantum mechanics, we move on to describe the two strong formalisms of classical mechanics, that are Hamiltonian and Lagrangian, very briefly. Finally, using all the tools, developing the theory of time propagators in Semi-classical mechanics, that will act as the rule of time evolution of the state vector in the phase space. Another Semi-classical

approximation called the WKB method is also discussed. Finally, a very simple model for electron interaction is discussed.

# Contents

# 1 Linear Algebra

Definitions of vectors and linear vector spaces are abstract, so to understand the key ideas we will restrict ourselves to 2 or 3 dimensional vectors (and vector spaces) as they are more familiar and easier to grasp. But, simultaneously we will try to develop the theory using abstract symbols (Dirac notations) so that we can easily generalise the theory to n dimensions and, furthermore to infinite dimensions.
We shall use objects like $|\psi\rangle$, $|\phi\rangle$, $|\chi\rangle$,... to represent vectors(In this notation, These vectors are called **ket vectors** or **kets**). It should be noted that even though we present most explanations in 2 or 3 dimensional spaces, we should really be thinking about all the ideas in an abstract n dimensional space.

## 1.1 Linear vector spaces (LVS)

Any object that satisfies certain relations, namely addition and scalar multiplication, in the following ways, is called a vector and is said to be a part of **linear vector space** $\mathbb{V}$.

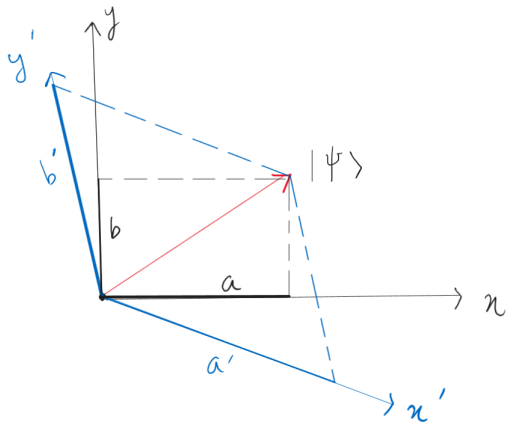
### Addition

- $|\psi\rangle + |\phi\rangle = |\phi\rangle + |\psi\rangle$
- $|\chi\rangle + (|\psi\rangle + |\phi\rangle) = (|\chi\rangle + |\psi\rangle) + |\phi\rangle$
- There exists a null vector $|\Omega\rangle$ such that $|\psi\rangle + |\Omega\rangle = |\psi\rangle$
- There exists a unique vector $-|\psi\rangle$ such that $|\psi\rangle + (-|\psi\rangle) = |\Omega\rangle$

### Scalar Multiplication

- $a|\psi\rangle \in \mathbb{V}\ \forall\ a \in \mathbb{R}$ or $\mathbb{C}$
- $a(b|\psi\rangle) = (ab)|\psi\rangle$
- $a(|\psi\rangle + |\phi\rangle) = a|\psi\rangle + a|\phi\rangle$
- $(a+b)|\psi\rangle = a|\psi\rangle + b|\psi\rangle$
- $1|\psi\rangle = |\psi\rangle$
- $0|\psi\rangle = |\Omega\rangle$

In this ket notations a vector should be understood as some abstract arrow, hanging around in an n dimensional space. Vector itself does not care as to *how* we describe it, but, description does depend on what basis we choose to expand it in. This will get clear from the following diagram.




The red vector $|\psi\rangle$ is something which is "out there", it is an abstract element of a LVS. Depending upon the basis *we* choose to represent it in, the components of the vector will change accordingly. The same $|\psi\rangle$ (for example) can be written as

$$|\psi\rangle \rightarrow a\,|x\rangle + b\,|y\rangle$$

Or

$$|\psi\rangle \rightarrow a'\,|x'\rangle + b'\,|y'\rangle$$

Note that basis need not be orthogonal, they just need to be linearly independent and span the space. While we are talking about these terms, we should define them a bit more rigorously.

## 1.2 Basis and dimensionality

A set of vectors $\{|\phi_k\rangle\,, k = 0, 1, 2, ...\}$ in a LVS forms a basis if it satisfies the following two requirements:

(a) All vectors in the set must be **linearly independent**. Formally, linear independence is defined as follows: If the only solution of the equation of kind $\sum_k c_k\,|\phi_k\rangle = 0$ is that all $c_k$'s are identically zero, then the set is said to be linearly independent.
In 2D vector space, two vectors are linearly dependent if they are collinear. In 3D, vectors can be linearly dependent if they are collinear like in 2D case but also if a 3rd vector is in the plane spanned by some other two linearly independent vectors, as the 3rd vector can be formed by scaling and adding the other two, so, in a sense, it is redundant. Although we can not visualise 4th or higher dimensional spaces but the idea is same. To form a linearly independent basis we need vectors that are all "quite different".

(b) Those basis vectors must be able to **span** the LVS, i.e., *every vector* $|\chi\rangle \in \mathbb{V}$ must be expressible as a linear combination of the basis: $|\chi\rangle = \sum_k b_k |\phi_k\rangle$

It should be noted that choice of basis is ours to make. Depending on different choices, the coefficients $b_k$'s will differ. The number of vectors in a basis (that spans the LVS) can be associated to the **dimensionality** of the LVS. For example, In TWO dimensional space, 2 linearly independent vectors can do the job (spanning the space), and similarly n linearly independent vectors can span some n dimensional LVS.

## 1.3 Dual of a LVS and Inner Products

Every LVS $\mathbb{V}$ has a **dual space** $\tilde{\mathbb{V}}$ that is also a LVS in of itself. The notation used for elements of $\tilde{\mathbb{V}}$ is $\langle\psi|, \langle\phi|, \langle\chi| ....$ These vectors are called **bra vectors**. The dual of $\tilde{\mathbb{V}}$ is again $\mathbb{V}$ itself, i.e., $\tilde{\tilde{\mathbb{V}}} = \mathbb{V}$.

The bilinear combination of a bra and a ket is called an **inner product**. It is a generalisation of dot products. Taking the bra vector $\langle\phi|$ for the dual space and the ket vector $|\psi\rangle$ from the original vector space. We form the inner product

$$\langle\phi|\psi\rangle \tag{1}$$

If the vector $|\psi\rangle$ in some basis is given by a $(n \times 1)$ column vector with complex entries $x_1, x_2, ..., x_n$, then the corresponding bra vector $\langle\psi|$ is given by the $(1 \times n)$ row vector ($x_1^*$ $x_2^*$ ... $x_n^*$). That is, if

$$|\psi\rangle = \begin{pmatrix} x_1 \\ x_2 \\ . \\ . \\ . \\ x_n \end{pmatrix} \tag{2}$$

Then

$$\langle\psi| = \begin{pmatrix} x_1^* & x_2^* & . & . & . & x_n^* \end{pmatrix} \tag{3}$$

It is easy to see that matrix multiplication of such a combination will give us a (complex) scaler. Let $a_i$'s and $b_i$'s be the elements of vector $|\phi\rangle$ and vector $|\psi\rangle$ respectively. Then

$$\langle\phi|\psi\rangle = \begin{pmatrix} a_1^* & a_2^* & . & . & . & a_n^* \end{pmatrix} \begin{pmatrix} b_1 \\ b_2 \\ . \\ . \\ . \\ b_n \end{pmatrix} = a_1^* b_1 + a_2^* b_2 + ... + a_n^* b_n \tag{4}$$

If $|\phi\rangle = |\psi\rangle$ then we get

$$\langle\psi|\psi\rangle = \sum_{i=1}^{n} |b_i|^2 \tag{5}$$

This is just like the expression for length squared that we are familiar with in real vector spaces and therefore the square root of this quantity is defined as the **norm** of a vector which is represented by

$$||\psi|| \equiv \langle\psi|\psi\rangle^{1/2} \tag{6}$$

Some general properties of inner products are as follows:

- $\langle\phi|\left(|\psi\rangle + |\chi\rangle\right) = \langle\phi|\psi\rangle + \langle\phi|\chi\rangle$
- $\left(\langle\psi + \phi|\right)|\chi\rangle = \langle\psi|\chi\rangle + \langle\phi|\chi\rangle$
- $\langle a\phi|b\psi\rangle = a^* b\,\langle\phi|\psi\rangle$
- $\langle\phi|\psi\rangle = \langle\psi|\phi\rangle^*$

## 1.4 Orthonormal basis sets

In our 3D space, we define a set of vectors $\hat{e_x}, \hat{e_y}$ and $\hat{e_z}$ that are all perpendicular to each other and their lengths are 1. This is an example of orthonormal basis. This idea can be generalised by looking at the relations of dot products between the three cartesian basis.

$$\hat{e_i} \cdot \hat{e_j} = \delta_{ij} \tag{7}$$

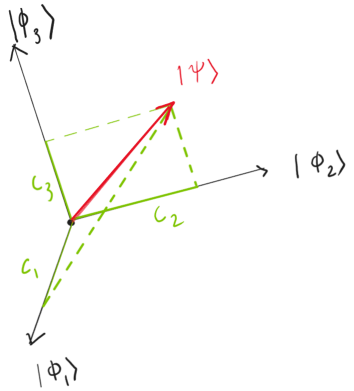
Where $i$ or $j$ can be $x, y$ or $z$ . The $\delta_{ij}$ symbol is **Kronecker delta** which is 1 if $i = j$ and 0 otherwise. This equation is just saying if $i = j$ (for example $\hat{e_x} \cdot \hat{e_x}$) the dot product is 1 and if we take the dot product of two orthogonal vectors, the dot product will be 0 (corresponding to the case $i \neq j$). In $n$ dimensions, if we have a basis set such that all $n$ vectors of the set are orthogonal to each other and with *norm* of each vector being unity, such a basis set is called an **orthonormal basis** $\{|\phi_k\rangle\}$.

$$\boxed{\langle\phi_j|\phi_k\rangle = \delta_{jk}} \quad (\textbf{orthonormality}) \tag{8}$$

### 1.4.1 Completness

### 1.4.2 Projection Operator

Consider a vector $|\psi\rangle$ in a 3 dimensional LVS expanded in an orthonormal basis $\{|\phi_i\rangle\}$. That is



$$|\psi\rangle = c_1 |\phi_1\rangle + c_2 |\phi_2\rangle + c_2 |\phi_2\rangle$$

Components of this vector $|\psi\rangle$ are NOT $c_i$ $(i = 1, 2, 3)$, because components of a vector are vectors, not scalars. Therefore, components of $|\psi\rangle$ are $c_i |\phi\rangle_i$. Note that $c_i$ can be found by taking the corresponding bra vector $\langle\phi_i|$ and 'hitting' $|\psi\rangle$ from the left, i.e.,

$$\langle\phi_i|\psi\rangle = \langle\phi_i| \left( \sum_{j=1}^{3} c_j |\phi_j\rangle \right) = \sum_{j=1}^{3} c_j \langle\phi_i|\phi_j\rangle = \sum_{j=1}^{3} c_j \delta_{ij} = c_i \tag{9}$$

Since the basis were orthogonal, only $c_i$ survived on the right hand side. Then, tacking on the corresponding $|\phi_i\rangle$, we can make the $i$th component $c_i |\phi_i\rangle$. So to find the **projection** of $|\psi\rangle$ in the direction of some $|\phi_i\rangle$, we do the following

$$\langle\phi_i|\psi\rangle |\phi_i\rangle = (|\phi_i\rangle \langle\phi_i|) |\psi\rangle = \hat{P}_i |\psi\rangle \tag{10}$$

Where

$$\hat{P}_i \equiv |\phi_i\rangle \langle\phi_i| \tag{11}$$

$\hat{P}_i$ is called the **Projection Operator** and we can see that it takes a vector$|\psi\rangle$ from right it spits out the projection of that vector along the vector $|\phi\rangle$.
Since $\hat{P}_i |\psi\rangle$ gives us the $i$th component, the sum over $i$ will be the sum of all three components of $|\psi\rangle$, which will give us $|\psi\rangle$ itself!

$$\sum_{i=1}^{3} \hat{P}_i |\psi\rangle = \left( \sum_{i=1}^{3} \hat{P}_i \right) |\psi\rangle = |\psi\rangle = I |\psi\rangle$$

$$\implies \sum_{i=1}^{3} \hat{P}_i = \sum_{i=1}^{3} |\phi_i\rangle \langle\phi_i| = I$$

This fact can be generalised to a LVS of any dimension $n$ to give us the result

$$\boxed{\sum_{i=1}^{n} |\phi_i\rangle \langle\phi_i| = I} \quad (\textbf{completeness}) \tag{12}$$

Note that Projection operators are actually $n \times n$ matrices (for finite $n$). As the ket vector is a column vector and bra vector is a row vector, it can be checked easily that the matrix multiplication of ket and bra will result in a matrix (While a matrix multiplication of bra and ket results in a scalar).

### 1.4.3 Gram-Schmidt orthonormalization

Given an arbitrary basis set, there is no guarantee that it is orthonormal, i.e., $\langle\phi_i.|\phi_j\rangle$ may be non zero for $i \neq j$. Usually it is better to work in a basis that is orthonormal so that we can exploit the properties such as orthonormality and completeness (given by eq(8) and eq(12) respectively). There exists a systematic process to transform any arbitrary

basis $\{|\psi_1\rangle, |\psi_2\rangle, ...\}$ into an orthonormal basis $\{|\phi_1\rangle, |\phi_2\rangle, ...\}$, that process is the **Gram-Schmidt orthonormalization**.

We will start simple. Let there be two linearly independent vectors $|\psi_1\rangle$ and $|\psi_2\rangle$ that are not orthonormal. We start with the first vector and divide it by its norm to normalise it.

$$|\phi_1\rangle = \frac{|\psi_1\rangle}{\langle\psi_1|\psi_1\rangle^{1/2}}$$

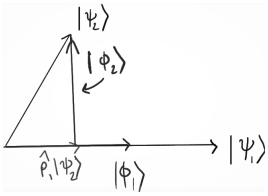
Then we subtract off the *projection* of $|\psi_2\rangle$ (onto $|\phi_1\rangle$) from itself, and normalise the result

$$|\phi_2\rangle = \frac{|\psi_2\rangle - \hat{P}_1 |\psi_2\rangle}{|| |\psi_2\rangle - \hat{P}_1 |\psi_2\rangle ||} = \frac{\left(I - \hat{P}_1\right)|\psi_2\rangle}{\langle\psi_2| \left(I - \hat{P}_1\right)|\psi_2\rangle^{1/2}}$$

where

$$\hat{P}_1 = |\phi_1\rangle \langle\phi_1|$$

The following diagram illustrates this idea.




If there was a third vector we would have subtracted off the projections of that $|\psi_3\rangle$ (on $|\phi_1\rangle$ and $|\phi_2\rangle$) from $|\psi_3\rangle$ and then normalised the result. This process can be continued for any number of vectors(given that oblique basis is linearly independent). We can find $|\phi_k\rangle$ as follows

$$|\phi_k\rangle = \frac{\left(I - \sum_{i=1}^{k-1} \hat{P}_i\right)|\psi_k\rangle}{\langle\psi_k| \left(I - \sum_{i=1}^{k-1} \hat{P}_i\right)|\psi_k\rangle^{1/2}} \tag{13}$$

## 1.5 Change of basis

Equation (12) will be very helpful for us, particularly to change basis, as we can insert identity anywhere and we can write identity as a sum of projection operators in any basis we want. Following example will make this idea more concrete.

Let $\{|\phi_k\rangle\}$ be an orthonormal basis in an LVS. Then any arbitrary element $|\psi\rangle$ of the LVS can be expanded in the form

$$\boxed{|\psi\rangle = \sum_j c_j |\phi_j\rangle} \quad \textbf{(expansion formula)} \tag{14}$$

Exploiting the orthogonality, $c_k$ is given by

$$\boxed{c_k = \langle\phi_k|\psi\rangle} \quad \textbf{(Inversion formula)} \tag{15}$$

Let there be another orthonormal basis set $|\chi_j\rangle$ so that

$$|\psi\rangle = \sum_k c_k |\phi_k\rangle = \sum_j d_j |\chi_j\rangle \tag{16}$$

We will start with $c_k$ and we will proceed by replacing identity operator by eq(12) using $|\chi_j\rangle$ in place of $|\phi_i\rangle$.

$$c_k = \langle\phi_k|\psi\rangle = \langle\phi_k|I|\psi\rangle = \langle\phi_k| \left( \sum_j |\chi_j\rangle \langle\chi_j| \right) |\psi\rangle$$

$$= \langle\phi_k| \sum_j |\chi_j\rangle \langle\chi_j|\psi\rangle = \sum_j \langle\phi_k|\chi_j\rangle \langle\chi_j|\psi\rangle$$

But from eq(16) $d_j = \langle\chi_j|\psi\rangle$, This gives

$$c_k = \sum_j d_j \langle\phi_k|\chi_j\rangle \tag{17}$$

Similarly

$$d_j = \sum_k c_k \langle\chi_j|\phi_k\rangle \tag{18}$$

These are the required change of basis formulas, further more let $|\Psi\rangle$ be another element of LVS, expanded in same basis

$$|\Psi\rangle = \sum_k C_k |\phi_k\rangle = \sum_j D_j |\chi_j\rangle \tag{19}$$

then

$$\langle\psi|\Psi\rangle = \sum_k c_k^* C_k = \sum_j d_j^* D_j$$

Setting $|\Psi\rangle = |\psi\rangle$

$$\boxed{||\psi||^2 = \sum_k |c_k|^2 = \sum_j |d_j|^2} \tag{20}$$

This is an example of **Parseval's Theorem**. This also implies that inner product of two vectors (and hence norm of a vector) is basis-independent (as it should be).

## 1.6 Matrices

When we think of a matrix, usually a box comes into mind, with some numbers written in it. It is helpful though to see matricx as an object that transforms a vector space. As always we can start by looking at a $2 \times 2$ matrix, the columns of this matrix encodes the information about the transformed versions of basis vectors. For example, a matrix such as

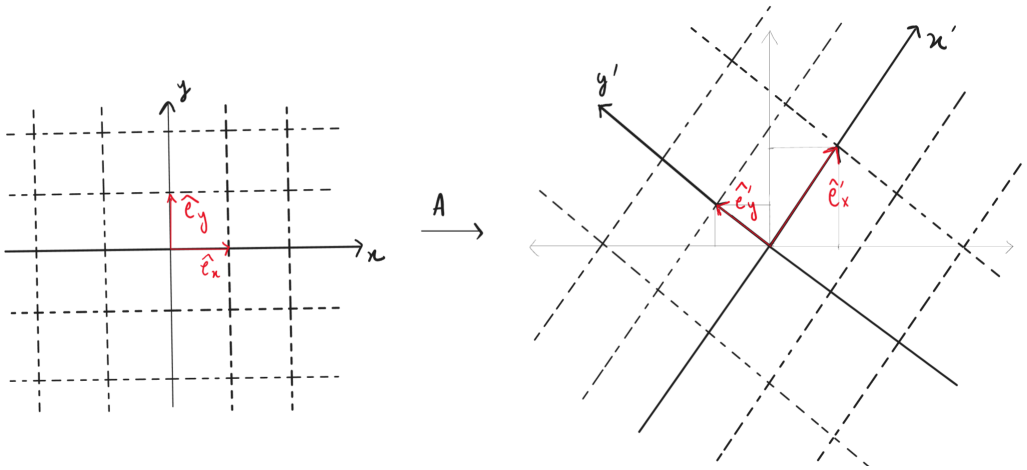
$$A = \begin{pmatrix} 1 & -1 \\ 2 & 1 \end{pmatrix}$$

It is a trivial matter to check that any column vector of dimensions $2 \times 1$ hitting this matrix from the right will result in another $2 \times 1$ column vector. It is in this sense we say

that matrices act on vectors to produce new vectors. If we see how a unit vector like $\hat{e_x}$ transforms, we will see that the result is just the first column of the matrix (and second column for $\hat{e_y}$). Since, any vector $(v_1, v_2)$ can be written as a linear combination of $\hat{e_x}$ and $\hat{e_y}$, knowing how the basis vectors transform is enough to know how will any vector transform.
If transformed $\hat{e_x}$ is $\hat{e'_x}$ and transformed $\hat{e_y}$ is $\hat{e'_y}$ then, transformed $\vec{v}$ is given by

$$\vec{v} = v_1\hat{e'_x} + v_2\hat{e'_y}$$

Every vector in the 2D space can be associated with a point whose coordinates are simply given by the components of the vector, A transformation such as $A$ can and does act on all such vectors (or points) to produce new vectors (or points), to keep track of where each of such point ends up after transformation, we can look at how *grid lines* of 2D space transform under the transformation. The transformation for the given example is shown in the figure below.




If we keep an original copy of the grid at the back ground we can see that location at which $\hat{e_x}$ ends up is actually the first column of the matrix $A$, i.e., $(1, 2)$, and $\hat{e_y}$ end up at $(-1, 1)$ which is the second column of the matrix $A$.
But just like the column representation of vectors this representation of a matrix can be converted to form including bra and ket notations, for this we note two things:

- Objects such as $|\phi_i\rangle \langle\phi_j|$ represents matrices

Let there two (orthonormal) basis vectors

$$|\phi_1\rangle = \begin{pmatrix}1\\0\end{pmatrix} \quad \text{and} \quad |\phi_2\rangle = \begin{pmatrix}0\\1\end{pmatrix}$$

then

$$|\phi_1\rangle \langle\phi_1| = \begin{pmatrix}1\\0\end{pmatrix}(1 \;\; 0) = \begin{pmatrix}1 & 0\\0 & 0\end{pmatrix}$$

similarly

$$|\phi_1\rangle \langle\phi_2| = \begin{pmatrix}0 & 1\\0 & 0\end{pmatrix}$$

$$|\phi_2\rangle \langle \phi_1| = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

$$|\phi_2\rangle \langle \phi_2| = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

These are called **natural basis** and now we can write any matrix $A$ as a linear combination of these 4 matrices, i.e.

$$A = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} = a_{11} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + a_{12} \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} + a_{21} \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} + a_{11} \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

$$= a_{11} |\phi_1\rangle \langle \phi_1| + a_{12} |\phi_1\rangle \langle \phi_2| + a_{21} |\phi_2\rangle \langle \phi_1| + a_{22} |\phi_2\rangle \langle \phi_2|$$

hence $A$ may be written as

$$\boxed{A = \sum_i \sum_j a_{ij} |\phi_i\rangle \langle \phi_j|} \tag{21}$$

- Matrix elements $a_{mn}$'s can be recovered by inserting $A$ between $\langle \phi_m|$ and $|\phi_n\rangle$.

$$\langle \phi_m|A|\phi_n\rangle = \langle \phi_m| \left( \sum_i \sum_j a_{ij} |\phi_i\rangle \langle \phi_j| \right) |\phi_n\rangle$$

$$= \sum_i \sum_j a_{ij} \langle \phi_m|\phi_i\rangle \langle \phi_j|\phi_n\rangle = \sum_i \sum_j a_{ij} \delta_{mi} \delta_{jn} = a_{mn}$$

hence

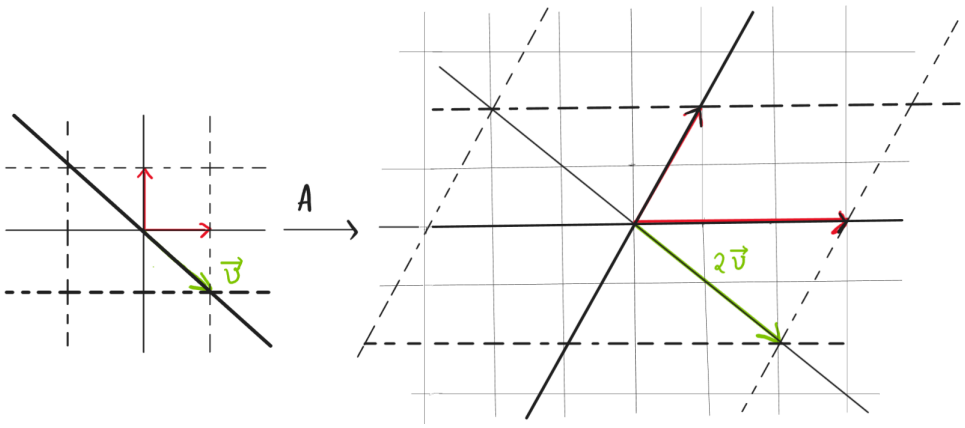
$$\boxed{a_{ij} = \langle \phi_i|A|\phi_j\rangle} \tag{22}$$

Equation(21) and (22) gives us a natural way to generalise matrices to infinite dimensions

## 1.7 Eigen vectors and Eigen values

To understand what eigen vectors are, we should first appreciate the fact that during a linear transformation most of the vectors do not stay on their spans (span of a single vector is just a line collinear with that vector). If a vector stays on its own span during a linear transformation, then that vector is called an **eigen vector** of that transformation.
For example, consider the transformation

$$A = \begin{pmatrix} 3 & 1 \\ 0 & 2 \end{pmatrix}$$




Note that the green vector $\vec{v}$ stayed on its own span after the transformation, It was just scaled by a factor of 2. Furthermore, the vector $\hat{e_x}$ also stayed on its span and was scaled by a factor of 3. These scalar factors by which an eigen vector scales is called the **eigen value** of that eigen vector. This transformation has two linearly independent eigen vectors

$$\begin{pmatrix} 1 \\ -1 \end{pmatrix} \quad \text{with eigen value 2}$$

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{with eigen value 3}$$

Note that if the dimensionality of a space is same as the number of linearly independent eigen vectors (of some transformation) in that space, we can choose these (normalised) eigen vectors as our basis, as they can span the space. By doing this we may loose some nice orthogonal properties of an orthonormal basis, but we can gain much more (as we will see later). Such basis are called **eigen basis**. Now we are in position to formally define an eigen vector.

If we apply some transformation $A$ on some vector $|\psi\rangle$ and the effect of that transformation is just that it scales the vector $|\psi\rangle$ by some amount $\lambda$, Then $|\psi\rangle$ is an eigen vector of transformation $A$ and $\lambda$ is eigen value of that vector.

$$A\,|\psi\rangle = \lambda\,|\psi\rangle \tag{23}$$

It follows immediately that

$$(A - \lambda I)\,|\psi\rangle = 0$$

Now there are two ways for this equation to hold true. One is the trivial case where $|\psi\rangle = 0$, but we are not interested in that. Other way is that the matrix $(A - \lambda I)$ is singular, i.e.,

$$\det(A - \lambda I) = 0 \tag{24}$$

In terms of transformations, this means for correct values of $\lambda$, the transformation corresponding to the matrix $A - \lambda I$ brings down the dimensionality of the space. For example, If a 3D space is collapsed to a plane, a line or a point, then the transformation is singular.

Fundamental theorem of algebra guarantees that an $n$th degree polynomial has $n$ roots in the complex field. From eq(24), we will get $n$ eigen values corresponding to an $n \times n$ matrix. This set of eigenvalues is called a **spectrum**. If the $n$ roots are not all unique, that is, some roots are repeated in the spectrum, the spectrum is said to be **degenerate**. In degenerate cases, a linear combination of two linearly independent eigen vectors can also be an eigen vector of the transformation, hence giving a whole "plane" of eigen vectors. But we may still be able to find an orthonormal basis using Gram-Schmidt orthonormalization procedure from a degenerate spectrum.

## 1.8 Important properties of matrices

### 1.8.1 Adjoint of a Matrix

Adjoint of a matrix (also called hermitian conjugate) is the transpose conjugate of that matrix. It is indicated by $A^\dagger$.

$$A^\dagger = \tilde{A}^* \tag{25}$$

If $|\psi\rangle$ and $\langle\phi|$ are elements of $\mathbb{V}$ and $\tilde{\mathbb{V}}$ respectively, Then it is easy to check (in orthogonal basis) that for a matrix $A$

$$\langle\phi|A\psi\rangle = \left\langle A^\dagger\phi\middle|\psi\right\rangle \tag{26}$$

### 1.8.2 Self Adjoint

If the hermitial conjugate of a square matrix is equal to the matrix itself, then the matrix is called **self adjoint** or **hermitian**:

$$A^\dagger = A \quad \text{Hermitian}; \qquad A^\dagger = -A \quad \text{skew hermitian} \tag{27}$$

One of the important properties of hermitian matrices is that their eigen values are guaranteed to be real. Let $\lambda$ be an eigen value of a hermitian matrix $A$: $A|\psi\rangle = \lambda|\psi\rangle$, then

$$\langle\psi|A\psi\rangle = \langle\psi|\lambda\psi\rangle = \lambda\langle\psi|\psi\rangle$$

but A is hermitan so

$$\langle\psi|A\psi\rangle = \langle A\psi|\psi\rangle = \langle\lambda\psi|\psi\rangle = \lambda^*\langle\psi|\psi\rangle$$

this gives

$$\lambda^* = \lambda$$

Hence, eigen values are real. Furthermore, Eigenvectors of hermitian transformation span the space and eigenvectors corresponding to different eigenvalues are **orthogonal**.

### 1.8.3 Unitary Transformations

When inverse of a matrix is equal to its hermitian conjugate, the matrix is said to be **unitary**:

$$U^\dagger = U^{-1} \tag{28}$$

A very important property of unitary transformations is that they preserve the inner products, and hence **preserve the norm** of a vector.

$$\langle U\phi|U\psi\rangle = \left\langle U^\dagger U\phi\middle|\psi\right\rangle = \left\langle U^{-1}U\phi\middle|\psi\right\rangle = \langle\phi|\psi\rangle$$

for $|\phi\rangle = |\psi\rangle$ we get preservation of norm. This is important because when we study quantum mechanics, norm of the state vector is related to the probability of finding the particle in space, which should stay 1 for all times, hence operators in quantum mechanics are unitary in nature.

### 1.8.4 Commutator

Matrix multiplication is not, in general, commutative ($AB \neq BA$), the *difference* between the two orderings is called the **commutator**:

$$[A, B] = AB - BA \tag{29}$$

Note that commutator of two matrices is also a matrix. Two identities involving commutators are:

$$[A + B, C] = [A, C] + [B, C] \tag{30}$$

$$[AB, C] = A[B, C] + [A, C]B \tag{31}$$

Caution: Order matters with matrices.
We mention that commuting matrices have this brilliant property that they are **simultaneously diagnolizable**, i.e., we can find a common set of eigen vectors for both the matrices *even* in degenerate cases.

## 1.9 The exponential of a matrix : $e^A$

Matrix exponentiation occurs frequently in physical applications. In a very broad sense, there is a good reason to regard *exponentiation of an operator* as the central problem of mathematical physics.

For example, while solving a system of linear first order differential equations with constant coefficients, we can model the problem such that solution is a trajectory in some abstract phase space, and equations are combined to make a vector equation of form:

$$\frac{d}{dt}\boldsymbol{x}(t) = A\boldsymbol{x}(t) \tag{32}$$

where (Let's assume for now) $A$ is a matrix with constant coefficients, then the solution (given the necessary and sufficient initial conditions) is:

$$\boldsymbol{x}(t) = e^{At}\boldsymbol{x}(0)$$

Other example (that we will discuss in detail later on) is from quantum mechanics itself: Given a system with time-independent Hamiltonian $H$, the time evolution of the physical observables pretaining to the system is governed by its time-development operator $e^{-iHt/\hbar}$

Another example is as follows: The Taylor series expansion of a function $f(x)$ at a point $x + a$ is given by

$$f(x + a) = f(x) + af'(x) + \frac{a^2}{2!}f''(x) + ... = e^{a(d/dx)}f(x)$$

Here, again we see that exponentiation of an operator ($a\frac{d}{dx}$) does the job of *translation* of the argument $x$ by the amount $a$.

$e^A$ is defined by the Taylor series of $e^x$ as follows:

$$\boxed{e^A \equiv I + A + \frac{A^2}{2!} + ... = \sum_{n=0}^{\infty} \frac{A^n}{n!}} \tag{33}$$

Note that if $A$ and $B$ are matrices, then it is not necessary that $e^A e^B = e^{A+B}$. This equality only holds when $A$ and $B$ *commute*. In fact, if $A$ and $B$ do not commute but they *do* commute with their commutator, i.e., $[A, [A, B]] = [B, [A, B]] = 0$, then

$$e^{A+B} = e^A e^B e^{-[A,B]/2} \tag{34}$$

This is known as **Baker-Campbell-Hausdroff formula**. This is easy to see that if $[A, B] = 0$, we get back our old, more familiar, identity.

# 2 Quantum Mechanics

Before laying down the foundations of quantum mechanics, I would like to introduce Infinite dimensional linear vector spaces and the idea of a continuous basis. Perhaps I should have covered these topics in the previous section which was dedicated to linear algebra but I think transition to quantum mechanics will be more natural this way.

## 2.1 The space $\ell_p$

The space $\ell_p$, where $p \geq 1$, is defined as comprising all infinite sequences that satisfy the condition

$$\left( \sum_{n=1}^{\infty} |x_n|^p \right)^{1/p} < \infty \tag{35}$$

The left hand side is called the $\ell_p$ norm of the vector. The dual of this space is the space $\ell_q$ such that

$$\frac{1}{p} + \frac{1}{q} = 1$$

For $\ell = 2$ we get a special case when the space $\ell_2$ becomes *self dual*, and it is called the space of **square-summable sequences**, i.e.,

$$\sum_{n=1}^{\infty} |x_n|^2 < \infty \tag{36}$$

Just like in the case of finite dimensions, we can think of vectors as column vectors or lists of infinite numbers, but this time, that list has infinite components:

$$|\psi\rangle = \begin{pmatrix} x_1 \\ x_2 \\ . \\ . \\ . \end{pmatrix} \quad , \quad |\phi\rangle = \begin{pmatrix} y_1 \\ y_2 \\ . \\ . \\ . \end{pmatrix}$$

The convergence condition in eq(39) ensures that the following inner product exists and is always finite

$$\langle \phi | \psi \rangle = \sum_{n=1}^{\infty} y_n^* x_n \tag{37}$$

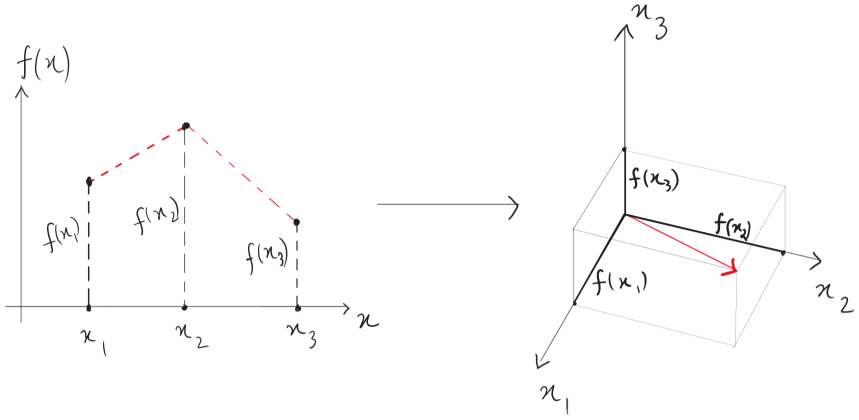
Setting $|\psi\rangle = |\phi\rangle$, we get the norm of the vector

$$||\psi||^2 = \langle \psi | \psi \rangle = \sum_{n=1}^{\infty} |x_n|^2 < \infty \tag{38}$$

## 2.2 Continuous basis

### 2.2.1 Functions as vectors

We will now try to see functions of single variables as vectors in an infinite dimensional space. We start simple and think about a function $f$ with a *discretized* input line $x$ with just three input points $x_1$, $x_2$ and $x_3$. Corresponding output values (or heights) are just $f(x_1)$, $f(x_2)$ and $f(x_3)$. See the figure below.




Now, we may think about this function as a vector in 3D space, with three orthogonal axes representing $x_1$, $x_2$ and $x_3$. Components of this vector are $f(x_1)$, $f(x_2)$ and $f(x_3)$.

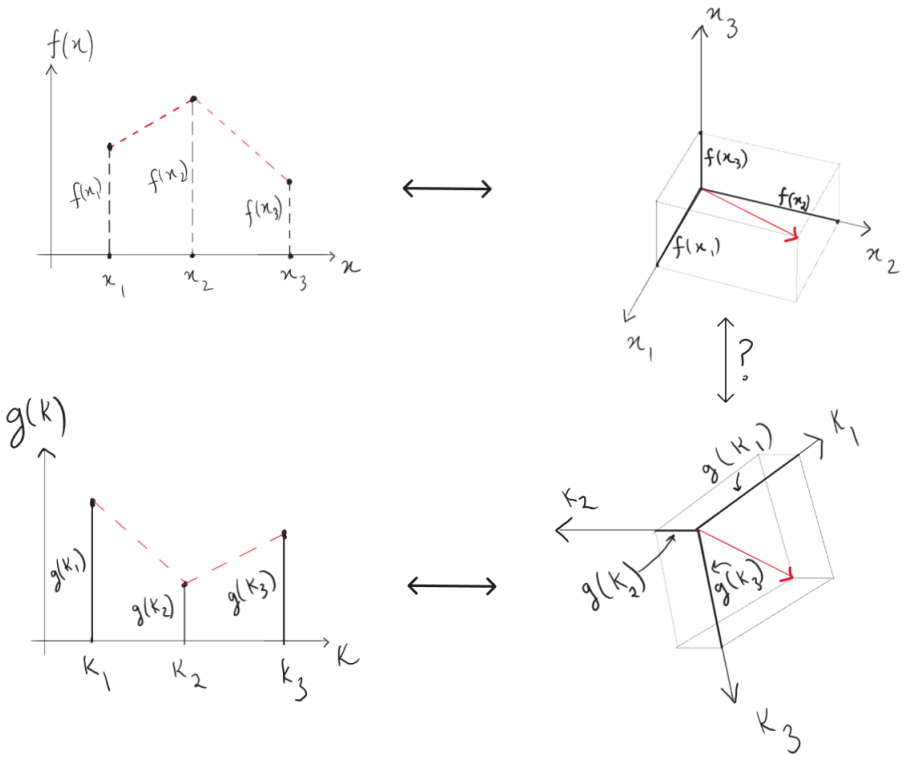
$$|f\rangle = f(x_1)\,|x_1\rangle + f(x_2)\,|x_2\rangle + f(x_3)\,|x_3\rangle \rightarrow \begin{pmatrix} f(x_1) \\ f(x_2) \\ f(x_3) \end{pmatrix}$$

Any function can be represented in this way as long as it has three discrete input points and 3 output points. Now we increase the resolution of the graph and allow for more $x_n$'s. We can represent such a function in a similar way in an $n$ dimensional vector space with components representing heights $f(x_n)$'s, i.e.,

$$|f\rangle = \sum_{j=1}^{n} f(x_j)\,|x_j\rangle = \begin{pmatrix} f(x_1) \\ f(x_2) \\ . \\ . \\ f(x_n) \end{pmatrix} \tag{39}$$

The final jump is to let $n \to \infty$ and instead of using some discrete index like $j$ to *label* the basis, we use a *symbol* like $x$ itself to label different orthogonal basis. Jumping from one input value $x_1$, to some other input $x_2$, corresponds to jumping from one axis $x_1$ to some other axis $x_2$ (remember that $x_1$ and $x_2$ are representing orthogonal *axes*). So the $x$ number line can be thought of as a set of *orthogonal* axes in an infinite dimensional space. Each axis representing a number on the $x$ line and vice-versa. In this way, any *continuous* function can be though of as a *vector* in this infinite dimensional vector space where orthogonal basis are changing *smoothly* from one axis to other. In this sense, we can say that value of $f(x)$ for *each* given value of the argument $x$ represents a 'component' of an abstract vector $|f\rangle$.

Now, we will go back to 3 dimensions to appreciate the fact that the *same* information that the function $f(x)$ is providing, can be provided in some different basis as well! See the figure below:




Here, we changed the basis (from $|x\rangle$ basis to $|k\rangle$ basis) without changing the vector representing the function $f$. The **components** $g(k_n)$'s encode the information about the same vector $f$ but in some other basis, hence if we translate back to the "graphing space" (bottom left), the *graph* corresponding to the vector $|g\rangle$ (which is same as the *vector* $|f\rangle$), may look a bit different then the *graph* of $f$. Hence we can say that same information can be provided and interpreted in various ways. Such change of basis of a vector in infinite dimensional vector space constitutes a **transformation**. We just need the rule that tells us how to change the basis. **Fourier Transforms** are an example of such change of basis from *time*

domain to *frequency* domain.

### 2.2.2 Completeness and orthonormality

. Analogs of eq(8), eq(12), eq(14) and eq(15) in a continuous basis are as follows:

$$\langle x'|x\rangle = \delta(x'-x) \quad \textbf{(orthonormality)} \tag{40}$$

Here $\delta(x-a)$ is the **Dirac delta function**. Technincally, it is a generalised function or distribution. This function of $x$ is zero everywhere except at $x=a$, where it is $\infty$. It looks like an infinitely high spike at $a$. The two key properties of this function are as follows:

- Area under this function is defined to be 1, i.e.,

$$\int_{-\infty}^{\infty} \delta(x-a)dx = 1 \tag{41}$$

- $$\int_{-\infty}^{\infty} f(x)\delta(x-a)dx = f(a) \tag{42}$$

The reason why Dirac delta function occurs in continuous basis orthonormality condition instead of the Kronecker delta can be understood once we state the completeness.

$$\int_{-\infty}^{\infty} dx\,|x\rangle\langle x| = I \quad \textbf{(completeness)} \tag{43}$$

If we see the effect of hitting a basis ket $|\phi_j\rangle$ from the right onto a complete set of basis, we get $|\phi\rangle$ back:

$$I\,|\phi_j\rangle = \left(\sum_i |\phi_i\rangle\langle\phi_i|\right)|\phi_j\rangle = \sum_i |\phi_i\rangle\,(\langle\phi_i|\phi_j\rangle) = \sum_i \delta_{ij}\,|\phi_i\rangle = |\phi_j\rangle$$

This should be replicated in continuous basis as well, which is guaranteed by eq(45) and eq(46) as follows

$$I\,|x\rangle = \left(\int_{-\infty}^{\infty} dx'\,|x'\rangle\langle x'|\right)|x\rangle = \int_{-\infty}^{\infty} dx'\,|x'\rangle\,(\langle x'|x\rangle) = \int_{-\infty}^{\infty} dx'\,|x'\rangle\,\delta(x'-x) = |x\rangle$$

Just like in finite dimensional cases, we can expand any *funciton* $f$ in terms of continuous orthonormal basis. For example:

$$|f\rangle = I\,|f\rangle = \left(\int_{-\infty}^{\infty} dx\,|x\rangle\langle x|\right)|f\rangle = \int_{-\infty}^{\infty} dx(\langle x|f\rangle)\,|x\rangle$$

$$\implies |f\rangle = \int_{-\infty}^{\infty} dx f(x)\,|x\rangle \quad \textbf{(expansion formula)} \tag{44}$$

where

$$\boxed{f(x) \equiv \langle x|f\rangle} \quad \text{and hence} \quad \langle f|x\rangle = f^*(x) \quad \textbf{(inversion formula)} \tag{45}$$

### 2.2.3 Hilbert Space

Note that this infinite dimensional space can be thought of as a natural continuum analog of the space $\ell_2$. It is also a self-dual LVS and the inner product of any two vectors $|f\rangle$ and $|g\rangle$ reduces to

$$\langle f|g\rangle \equiv \langle f| \left( \int_{-\infty}^{\infty} dx \, |x\rangle \langle x| \right) |g\rangle = \int_{-\infty}^{\infty} dx \, \langle f|x\rangle \langle x|g\rangle$$

hence

$$\boxed{\langle f|g\rangle = \int_{-\infty}^{\infty} f^*(x) g(x) dx} \quad \textbf{(inner product)} \tag{46}$$

for $|f\rangle = |g\rangle$,

$$||f||^2 = \langle f|f\rangle = \int_{-\infty}^{\infty} |f(x)|^2 dx \tag{47}$$

This integral, representing the norm, is less that $\infty$. There is a special name for this function space. It is called **the space of square-integrable functions** and it is denoted by $\mathcal{L}_2(-\infty, \infty)$.

In infinite dimensional LVS, doing some operation on an element vector of a LVS may take that vector out from the LVS. So it is of interest to talk about, for the sake of consistency, *subspaces* in infinite dimensional linear vector spaces and *domains* of operators in a LVS so that we stay in a subspace and do not wander off. To understand one such special self-dual subspace, We state the following two facts:

- A sequence of vectors $|\phi_n\rangle$, where $n = 1, 2, ..$ ad inf., is a **Cauchy Sequence** if the difference vector $|\phi_n\rangle - |\phi_m\rangle$ tends to the null vector $|\Omega\rangle$ as both $n$ and $m \to 0$.
- A LVS which includes all limit vectors of Cauchy sequences among its elements is said to be **complete linear space**.

A LVS in which the inner product is defined and which is *complete*, in the sense just described in the previous point, is called a **Hilbert space**. In quantum mechanics, we work in Hilbert spaces.

## 2.3 Postulates of quantum mechanics

Now with all the tools on table, we can start to talk about quantum mechanics freely. The postulates we mention here are related to the **Schrodinger picture**. There are other ways to interpret quantum mechanics, for example:

- The Heisenberg picture in which the operators do the job of evolution of expectation values.
- The interaction picture in which both, the state vector and the Operator can determine the time evolution. This picture is advantageous to use when the Hamiltonian has a first order explicit time dependence and an autonomous part. This picture, coined by Dirac, can separate the problems into two parts.

1. There exists a state vector $|\Psi(t)\rangle$ in an Infinite dimensional Hilbert space that encodes all the information about a system that can be known (or measured).

The idea of a vector holding information is not a quantum one. For example, we can think of the $N$-body problem in classical mechanics. Where $N$ massive bodies are moving around in 3D space effecting each others' motion. We can list the locations, momenta, spin components etc. in a column vector. The components of that column vector can tell us everything we want to know about the system. Those components can change with time. In general that abstract vector, that we call a state vector, may live in a very large (but finite) dimensional space. Knowing the *initial* state vector and some rule about the *time evolution* of that vector, we can predict what the state of the system is going to be at any arbitrary time in the future. The rules of time evolution maybe Newton's equations of motion, or Hamilton's equations etc. The jump in quantum mechanics is that this state vector lives in an infinite dimensional Hilbert space.

2. For every physical observable $A$, there exists a **self-adjoint operator** $\hat{A}$, acting upon vectors in the Hilbert space.

For example, the operator related to the total energy content of the system is the **Hamiltonian operator**. We shall talk more about Hamiltonian in later sections (see section 3.3 first if it is the preferable flow of the reader).
For simplicity, let us say that eigen value spectrum of $A$ is discrete. Eigen vectors are $|\phi_n\rangle$ and eigen values are $\lambda_n$. We expand the state vector $|\Psi(t)\rangle$ in the eigen basis of $\hat{A}$.

$$|\Psi(t)\rangle = \sum_n c_n(t)\,|\phi_n\rangle \tag{48}$$

If the basis are orthonormal, it follows from the inversion formula eq(45) that

$$c_n(t) = \langle\phi_n|\Psi(t)\rangle \tag{49}$$

Which leads us to the third postulate..

3. If $|\Psi(t)\rangle$ is normalised, then $|c_n(t)|^2$ is the probability that the measurement of $A$ at time $t$ will yield the corresponding eigenvalue $\lambda_n$ as the outcome of that measurement. If the eigen spectrum is continuous: $\lambda(x)$, then probability of getting a result in range $dx$ is $|c(x,t)|^2 dx$

Note that these eigen values $\lambda_n$ are guaranteed to be real because $\hat{A}$ is self-adjoint. It is also said that the system is in state $|\phi_n\rangle$ at time $t$ but this language is a bit hand-wavy, the system is *not* in $|\phi_n\rangle$ it is in a superposition state $|\Psi(t)\rangle$. It is that only after making a *measurement*, we find the system in some particular state, before that it is in the superposition of all $|\phi_n\rangle$'s *weighted* by $c_n(t)$, and anyway, we measure an observable $A$ , not the state of a system( State vector is an abstract complex vector in Hilbert space). These $c_n(t)$'s are called the **probability amplitudes**. The idea that the system *chooses* a state as soon as a measurement is made is called the **collapse** of the State vector. The question of the collapse is still one of the open questions of the quantum theory.

Furthermore, this probabilistic interpretation will help us find the *expectation value* of the observable $A$ by taking the weighted average. Since when in state $|\phi_n\rangle$, the measurement yields the value $\lambda_n$, we can say that

$$\langle A\rangle = \sum_n \lambda_n |c_n(t)|^2 = \sum_n \lambda_n c_n(t) c_n^*(t) = \sum_n \lambda_n \langle\phi_n|\Psi(t)\rangle \langle\Psi(t)|\phi_n\rangle$$

$$= \langle\Psi(t)| \left( \sum_n (\lambda_n |\phi_n\rangle) \langle\phi_n| \right) |\Psi(t)\rangle = \langle\Psi(t)| \left( \sum_n \hat{A} |\phi_n\rangle \langle\phi_n| \right) |\Psi(t)\rangle$$

$$= \langle\Psi(t)| \hat{A} \left( \sum_n |\phi_n\rangle \langle\phi_n| \right) |\Psi(t)\rangle = \langle\Psi(t)| \hat{A} I |\Psi(t)\rangle = \langle\Psi(t)|\hat{A}|\Psi(t)\rangle$$

Where in second line we have used the fact that $|\phi_n\rangle$ is an eigen state of $\hat{A}$ to write $\lambda_n |\phi_n\rangle$ as $\hat{A}|\phi_n\rangle$. Hence, expectation value of any observable at time $t$ can be found by *sandwiching* the operator corresponding to that observable between bra and ket of the state vector $|\Psi(t)\rangle$, i.e.,

$$\boxed{\langle A\rangle = \langle\Psi(t)|\hat{A}|\Psi(t)\rangle} \tag{50}$$

4. The operators corresponding to the position and momentum do NOT commute with each other.

Their commutator is given by

$$\frac{[\hat{r_i}, \hat{p_j}]}{i\hbar} = \delta_{ij} \tag{51}$$

Also

$$[\hat{r_i}, \hat{r_j}] = [\hat{p_i}, \hat{p_j}] = 0 \tag{52}$$

eq(51) and eq(52) put together make the **canonical commutation relations** in quantum mechanics. We have something similar in classical mechanics, where the **poisson brackets** (sect 3.3) of the conjugate variables $q$ and $p$ do not commute. Here, $q$ and $p$ are generalised coordinates, poisson bracket is defined as follows:

$$\{A, B\} = \sum_i \left( \frac{\partial A}{\partial q_i}\frac{\partial B}{\partial p_i} - \frac{\partial B}{\partial q_i}\frac{\partial A}{\partial p_i} \right)$$

and the corresponding canonical commutation relations are

$$\{q_i, p_j\} = \delta_{ij}$$

$$\{q_i, q_j\} = \{p_i, p_j\} = 0$$

We will talk more about these in the upcoming sections on Hamiltonian Dynamics. We mentioned the results here so that one can appreciate how the classical mechanics was naturally extended to quantum mechanics.

Note the role played by $i$ in the denominator of eq(54). Since, commutator of two physical observable will also be an observable, it is necessary for this commutator to be hermitian. But the commutator of two hermitian operators is NOT hermitian (in

fact it is skew-hermitian). To make the commutator hermitian, we introduced an $i$ in the denominator. Moreover, the $\hbar$ is there for dimensional reasons, because the dimensions of (position) $\times$ (momentum) is J-s, just like $\hbar$, introducing $i$ makes the whole commutator dimensionless.

5. The rule of time evolution of the state vector $|\Psi\rangle$ is given by the **Schrodinger's equation**:

$$\boxed{i\hbar\frac{d}{dt}|\Psi(t)\rangle = \hat{H}|\Psi(t)\rangle} \tag{53}$$

Of course, we need the initial state vector $|\Psi(t_0)\rangle$ to solve this first order equation (in time). $\hat{H}$ is the Hamiltonian of the system, the operator corresponding to the total energy content. For an *autonomous* Hamiltonian, i.e., Hamiltonian that does not depend *explicitly* on time (or to say only conservative forces are at play, causing energy conservation of the system). The formal solution to the Schrodinger's equation becomes

$$\boxed{|\Psi(t)\rangle = exp\left(\frac{-i\hat{H}(t-t_0)}{\hbar}\right)|\Psi(t_0)\rangle} \tag{54}$$

Note that if $|\Psi(t_0)\rangle$ was normalised, i.e., $\langle\Psi(t_0)|\Psi(t_0)\rangle = 1$, then

$$\langle\Psi(t)|\Psi(t)\rangle = \langle\Psi(t_0)|\, exp\left(\frac{i\hat{H}(t-t_0)}{\hbar}\right) exp\left(\frac{-i\hat{H}(t-t_0)}{\hbar}\right)|\Psi(t_0)\rangle$$

We did not change $H$ to $H^\dagger$ (as suggested by eq(26)) while taking the ad-joint as it is self-adjoint, and that is because it corresponds to a physical observable (total energy). Now, the operators in the middle should be given proper care. Using the formula $e^A e^B = e^{A+B}e^{-[A,B]/2}$ from eq(34) and using the fact that any operator commutes with it's negative, i.e., $[\hat{A}, \hat{-A}] = 0$. So we can use the simpler formula $e^A e^B = e^{A+B}$. Let

$$U(t,t_0) \equiv exp\left(\frac{i\hat{H}(t-t_0)}{\hbar}\right)$$

$$exp\left(\frac{i\hat{H}(t-t_0)}{\hbar}\right) exp\left(\frac{-i\hat{H}(t-t_0)}{\hbar}\right) = UU^\dagger = I$$

$$\implies \text{If} \quad \langle\Psi(t_0)|\Psi(t_0)\rangle = 1 \quad \text{then,} \quad \langle\Psi(t)|\Psi(t)\rangle = 1 \tag{55}$$

Hence, we establish that the norm of state vector $|\Psi(t)\rangle$ is preserved in time. That means the probability of its existence in all space is conserved in time. Once a state is normalised, it stays normalised. This is a consequence of the fact the $U(t,t_0)$ is **Unitary**, which is consistent with what we saw in sect 1.8.3 that unitary transformations preserve the norm.

We get the result for this special case of autonomous Hamiltonian that $U(t,t_0)$ is Unitarty and it is called the **time evolution operator**. In quantum mechanics unitarity of the time evolution operator plays a crucial role even in more general systems.

## 2.4 The Schrodinger's equation

### 2.4.1 Position eigen basis

Position eigen kets are defined in the usual way:

$$\hat{x}\,|x_0\rangle = x_0\,|x_0\rangle$$

Here, $\hat{x}$ is operator associated with position, $|x_0\rangle$ is the eigen vector, and $x_0$ is the corresponding eigen value. Along with this we have the orthonormality condition (eq(40)):

$$\langle x'|x\rangle = \delta(x'-x)$$

We can write the state vector $|\Psi(t)\rangle$ by hitting it with a complete set of states from left:

$$|\Psi(t)\rangle = I\,|\Psi(t)\rangle = \left(\int_{-\infty}^{\infty} dx'\,|x'\rangle\,\langle x'|\right)|\Psi(t)\rangle = \int_{-\infty}^{\infty} dx'\,\langle x'|\Psi(t)\rangle\,|x'\rangle$$

we define the coefficient $\langle x'|\Psi(t)\rangle$ as $\psi(x',t)$ where $t$ dependence is from the state vector. Hence, the *overlap* of the state vector $|\Psi(t)\rangle$ with a position eigenket $|x\rangle$ i given by

$$\langle x|\Psi(t)\rangle = \langle x|\left(\int_{-\infty}^{\infty} dx'\psi(x',t)\,|x'\rangle\right) = \int_{-\infty}^{\infty} dx'\psi(x',t)\,\langle x|x'\rangle$$

$$= \int_{-\infty}^{\infty} dx'\psi(x',t)\delta(x-x') = \psi(x,t)$$

We get the result

$$\boxed{\langle x|\Psi(t)\rangle = \psi(x,t)} \tag{56}$$

Since, $\psi(x,t)$ is the expansion coefficient, hence from postulate (3), $|\psi(x,t)|^2dx$ is the probability of finding the particle between the position $x$ and $x+dx$.

### 2.4.2 Momentum operator in position eigen basis

We start with postulate (4), i.e.,

$$[\hat{x},\hat{p}] = i\hbar$$

Note that I have abbreviated $\hat{p_x}$ as just $\hat{p}$. Next, we sandwich this operator between $\langle x|$ and $|x\rangle$:

$$\langle x|(\hat{x}\hat{p}-\hat{p}\hat{x})|x'\rangle = \langle x|i\hbar|x'\rangle = i\hbar\,\langle x|x'\rangle = i\hbar\delta(x-x')$$

On the LHS, $\hat{x}$ can act on $|x'\rangle$ to produce $x'\,|x'\rangle$ as $|x'\rangle$ is an eigen vector of position operator $\hat{x}$. Similarly $\langle x|\,\hat{x}$ will produce $x^*\,\langle x|$, but since $x^* = x$ (eigen values of $\hat{x}$ should be real as it is a hermitian operator).Beware that $\hat{x}$ is an operator while $x$ is just a scalar number. This gives us

$$(x-x')\,\langle x|\hat{p}|x'\rangle = i\hbar\delta(x-x') \implies \langle x|\hat{p}|x'\rangle = \frac{\delta(x-x')}{(x-x')}$$

Using the fact that derivative of the delta function is negative of delta function divided by $x$:

$$\frac{d}{dx}\delta(x) = -\frac{\delta(x)}{x}$$

We get

$$\langle x|\hat{p}|x'\rangle = -i\hbar\frac{\partial}{\partial x}\delta(x-x') = -i\hbar\frac{\partial}{\partial x}\langle x|x'\rangle$$

Finally, expanding any arbitrary state vector $|\Psi(t)\rangle$ in $|x'\rangle$ basis and using the above equation, we can show that

$$\langle x|\hat{p}|\Psi(t)\rangle = -i\hbar\frac{\partial}{\partial x}\langle x|\Psi(t)\rangle \tag{57}$$

This gives us the position space representation of momentum operator:

$$\boxed{\hat{p} \to -i\hbar\frac{\partial}{\partial x}} \tag{58}$$

### 2.4.3 Momentum eigen functions in position basis

We start with defining the eigen value equation for the momentum eigen states $|p_0\rangle$ in the usual manner:

$$\hat{p}\,|p_0\rangle = p_0\,|p_0\rangle$$

To find position eigenkets in position basis we hit both sides of the previous equation from left by $\langle x|$:

$$\langle x|\hat{p}|p_0\rangle = p_0\,\langle x|p_0\rangle$$

But using eq(58) we can right the L.H.S as

$$-i\hbar\frac{\partial}{\partial x}\langle x|p_0\rangle = p_0\,\langle x|p_0\rangle$$

Hence, we get (apart from a constant) $\langle x|p_0\rangle$ to be equal to

$$\boxed{\langle x|p_0\rangle \propto e^{ip_0x/\hbar}} \tag{59}$$

Therefore,

$$\langle p_0|x\rangle = \langle x|p_0\rangle^* \propto e^{-ip_0x/\hbar} \tag{60}$$

### 2.4.4 Fourier Transforms

Using the results from previous seciton, we can change the basis for $\psi(x,t)$ as follows:

$$\psi(x,t) = \langle x|\Psi(t)\rangle = \langle x|\left(\int_{-\infty}^{\infty} dp\,|p\rangle\,\langle p|\right)|\Psi(t)\rangle = \int_{-\infty}^{\infty} dp\,\langle x|p\rangle\,\langle p|\Psi(t)\rangle$$

defining $\langle p|\Psi(t)\rangle \equiv \tilde{\psi}(p,t)$ (reason for the choice of this symbol will be obvious in a minute) and using eq(59):

$$\psi(x,t) \propto \int_{-\infty}^{\infty} dp\ \tilde{\psi}(p,t)e^{ipx/\hbar}$$

Similarly, we could have started by defining $\langle p|\Psi(t)\rangle$ first as we did in section 2.4.1 and found inverse result, i.e.,

$$\tilde{\psi}(p,t) \propto \int_{-\infty}^{\infty} dp\ \psi(x,t)e^{-ipx/\hbar}$$

$\psi(x,t)$ and $\tilde{\psi}(p,t)$ are called **Position space wave function** and **Momentum space wave function** respectively, and as we can see that they are **Fourier Transforms** of each other. The interpretation for the later is similar to that of former. $|\tilde{\psi}(p,t)|^2 dp$ is the probability that particle will have momentum in the range $dp$. Removing the proportionality sign by using an appropriate constant and generalising for 3 dimensions we get:

$$\boxed{\psi(\boldsymbol{r},t) = \frac{1}{(2\pi\hbar)^{3/2}} \int e^{-i(\boldsymbol{p}\cdot\boldsymbol{r})} \tilde{\psi}(\boldsymbol{p},t) d^3\boldsymbol{r}} \tag{61}$$

$$\boxed{\tilde{\psi}(\boldsymbol{p},t) = \frac{1}{(2\pi\hbar)^{3/2}} \int e^{i(\boldsymbol{p}\cdot\boldsymbol{r})} \psi(\boldsymbol{r},t) d^3\boldsymbol{p}} \tag{62}$$

where, $\boldsymbol{p}$ operator (in position basis) is given by

$$\boldsymbol{p} \to -i\hbar\nabla \tag{63}$$

Here, the gradient operator $\nabla$ is defined in it's usual way:

$$\nabla \equiv \left( \hat{\boldsymbol{x}} \frac{\partial}{\partial x} + \hat{\boldsymbol{y}} \frac{\partial}{\partial y} + \hat{\boldsymbol{z}} \frac{\partial}{\partial z} \right) \quad \text{(in Cartesian coordinates)}$$

### 2.4.5 Schrodinger's equation for a single particle

For a particle, of mass $m$, in some potential $V(\boldsymbol{r})$, the (autonomous) Hamiltonian operator is given by

$$\hat{H} = \frac{\hat{p}^2}{2m} + \hat{V}(\boldsymbol{r}) \tag{64}$$

Hence, Schrodinger's equation reads:

$$i\hbar \frac{d}{dt} |\Psi(t)\rangle = \left( \frac{\hat{p}^2}{2m} + \hat{V}(\boldsymbol{r}) \right) |\Psi(t)\rangle \tag{65}$$

It is use full to write this equation in position basis because we do not know how horrible the potential operator $\hat{V}$ is in it's form. Taking the position projection will make this V a scalar function of $\boldsymbol{r}$ regardless of it's form because the V operator is a function of position itself.

$$i\hbar \frac{d}{dt} \langle \boldsymbol{r}|\Psi(t)\rangle = \frac{1}{2m} \langle \boldsymbol{r}|\hat{p^2}|\Psi(t)\rangle + \langle \boldsymbol{r}|\hat{V}(\boldsymbol{r})|\Psi(t)\rangle$$

using eq(66) to replace $\hat{p}$ in position basis, and eq(59), we get:

$$\boxed{i\hbar \frac{d}{dt} \psi(\boldsymbol{r},t) = -\frac{\hbar^2}{2m} \nabla^2 \psi(\boldsymbol{r},t) + V(\boldsymbol{r}) \psi(\boldsymbol{r},t)} \tag{66}$$

Normalisation condition becomes:

$$\int d^3\boldsymbol{r} |\psi(\boldsymbol{r},t)|^2 = 1 \tag{67}$$

Where $\psi(\boldsymbol{r},t)$ belongs to $\mathcal{L}_2(-\infty,\infty)$.

### 2.4.6 Separation of temporal part in Schrodinger's equation

We can expand $|\Psi(t)\rangle$ in the eigen basis of the Hamiltonian so that

$$\hat{H}\,|\Phi(t)\rangle = E\,|\Phi(t)\rangle \tag{68}$$

Here, $|\Phi(t)\rangle$ is the eigen vector of operator $\hat{H}$ with $E$ being the corresponding eigenvalue. Hence we can write the Schrodinger's equation as

$$i\hbar\frac{d}{dt}\,|\Phi(t)\rangle = E\,|\Phi(t)\rangle$$

Then the solution is

$$|\Phi(t)\rangle = e^{-iEt/\hbar}\,|\Phi(0)\rangle \tag{69}$$

Therefore, Schrodinger's equation is solved trivially for an eigen state of the Hamiltonian. If we can expand a general state vector $|\Psi(t)\rangle$ in terms of the eigen state of the Hamiltonian, then we can write the general solution as:

$$\Psi(t) = \sum_n c_n\,|\Phi_n(t)\rangle = \sum_n c_n e^{-iE_nt/\hbar}\,|\Phi_n(0)\rangle \tag{70}$$

where $n$ is incorporates all the quantum numbers that can come up while solving for $|\Phi_n(t)\rangle$'s, i.e., solving the *eigenvalue equation* in eq(68). We may also write the same equation in position basis where we get:

$$\hat{H}\phi_n(x) = E_n\phi_n(x) \tag{71}$$

where $\phi_n(x)$ are the energy eigen functions *in* position basis. with the solutions

$$\phi_n(x,t) = e^{-iE_nt/\hbar}\phi_n(x,0) \tag{72}$$

Such states are called **Stationary states** because expectation value of any observable stays constant with time, as we may see that

$$\langle A\rangle_t = \int \phi_n^*(x,t)\hat{A}\phi_n(x,t)dx = \int e^{iE_nt/\hbar}\phi_n^*(x,0)\hat{A}e^{-iE_nt/\hbar}\phi_n(x,0)dx$$

$$= \int \phi_n^*(x,0)\hat{A}\phi_n(x,0) = \langle A\rangle_0$$

## 2.5 Annihilation and creation operators

In treating the case for a quantum harmonic oscillator, Dirac used a method in which we factorise the Hamiltonian in $\hat{x}$ and $\hat{p}$. Hamiltonian of harmonic oscillator is a very symmetric one:

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}mw^2\hat{x}^2 \tag{73}$$

We define the following operators:

$$a = \frac{\hat{x}}{\sqrt{2\hbar/mw}} + \frac{i\hat{p}}{\sqrt{2mw\hbar}} \tag{74}$$

and it's adjoint:

$$a^\dagger = \frac{\hat{x}}{\sqrt{2\hbar/mw}} - \frac{i\hat{p}}{\sqrt{2mw\hbar}} \tag{75}$$

Furthermore

$$[a, a^\dagger] = 1 \tag{76}$$

These are called the **ladder operators** or **Annihilation** and **creation operators**. Reason will reveal itself once we consider the following operator and its eigenvalues:

$$N \equiv a^\dagger a$$

and following commutation relations hold (using the definition of $a$ and $a^\dagger$ with eq(31))

$$[N, a] = -a \tag{77}$$

$$[N, a^\dagger] = a^\dagger \tag{78}$$

If we use $|\lambda\rangle$ to label the eigenkets of $N$ operator, then

$$N|\lambda\rangle = \lambda|\lambda\rangle$$

If we see the effect of $[N, a]$ on an eigenket, we see

$$[N, a]|\lambda\rangle = -a|\lambda\rangle$$

$$\implies Na|\lambda\rangle - aN|\lambda\rangle = -a|\lambda\rangle$$

$$\implies N(a|\lambda\rangle) = (\lambda - 1)a|\lambda\rangle$$

Hence, if $|\lambda\rangle$ is an eigenket with eigenvalue $\lambda$, so is $a|\lambda\rangle$ with eigen value $(\lambda - 1)$. Similar treatment with $[N, a^\dagger]$ will give us that if $|\lambda\rangle$ is an eigenket with eigenvalue $\lambda$, then so is $a^\dagger|\lambda\rangle$ with eigen value $(\lambda + 1)$.
Hence, $a^\dagger$ *raises* the eigenvalue by 1 while $a$ lowers it by 1. But since expectation value of $N$ should be always positive (as $\langle N\rangle = \langle a^\dagger a\rangle = \langle\Psi|a^\dagger a|\Psi\rangle = ||a\Psi||^2$). Therefore we say that there exists a state $|0\rangle$ such that upon lowering it we get 0, i.e.,

$$a|0\rangle = 0 \tag{79}$$

Hence, $\lambda$'s must be natural numbers. We identify these eigen states by writing $|n\rangle$ where $n = 0, 1, 2, ....$ If we normalise these states, the following relations can be found:

$$\langle n|n\rangle = 1$$

$$a^\dagger a|n\rangle = N|n\rangle = n|n\rangle$$

$$a^\dagger|n\rangle = \sqrt{n+1}\,|n+1\rangle \quad \text{(Creation)} \tag{80}$$

$$a|n\rangle = \sqrt{n}\,|n-1\rangle \quad \text{(Annihilation)} \tag{81}$$

We can immediately solve the quantum harmonic oscillator using these. The hamiltonian becomes

$$\hat{H} = \hbar w\left(N + \frac{1}{2}\right) \tag{82}$$

We mention the fact that the energy spectrum is equally spaced (Such states belong to a family of **Isospectral states**).

$$E_n = \hbar w \left( n + \frac{1}{2} \right) \tag{83}$$

Ground state $|0\rangle$ in position eigen basis Turns out to be a Gaussian function and the excited states are created by applying creation operator on the *vacuum* $|0\rangle$. In position basis, energy eigen functions are **Hermite polynomials** weighted by a Gaussian. One of the interesting features is that $|0\rangle$ hits the uncertainty saturation, i.e.

$$\sigma_x \sigma_p = \frac{\hbar}{2}$$

It is an example of a **Coherent state**. More about this topic in next subsection.

### 2.5.1 Coherent states

If we write down the annihilation and creation operators in units where the physical constants are unity (we can always put them back at any stage we like) we get:

$$a = \frac{x + ip}{\sqrt{2}}$$

$$a^\dagger = \frac{x - ip}{\sqrt{2}}$$

Asking about the eigenstates of $a$ or $a^\dagger$, it turns out that $a^\dagger$ does not have any normalizable eigenstates, but $a$ does. Let $|\alpha\rangle$ be an eigenstate of $a$ then it turns out that

$$a\,|\alpha\rangle = e^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle \tag{84}$$

where $|n\rangle$ are eigenstates of $N$ operator and $\alpha$ is the corresponding eigenvalue. Finally, using the fact that

$$|n\rangle = \frac{(a^\dagger)^n}{\sqrt{n!}} |0\rangle \tag{85}$$

We can write $|\alpha\rangle$ as

$$|\alpha\rangle = e^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{(\alpha a^\dagger)^n}{n!} |0\rangle \tag{86}$$

We can write this more compactly as

$$\boxed{|\alpha\rangle = e^{\alpha a^\dagger - \alpha^* a} |0\rangle} \quad \textbf{(Coherent states)} \tag{87}$$

We again see the exponentiation of an operator. Anyway, the effect of the operator on $|0\rangle$ is in someways just to shift the centre of oscillation of the oscillator. All coherent state are minimum uncertainty states.

## 2.6 Uncertainty Principle

We will mention some more important facts of quantum mechanics in this section itself. Starting with uncertainty principle.
By uncertainty, we mean the *standard deviation* in the outcomes of a measurement. The crucial input to finding a general is a fact about Hilbert space that is called **Schwarz inequality**, which states that:

$$|\langle\phi|\psi\rangle|^2 \leq \langle\phi|\phi\rangle\langle\psi|\psi\rangle \quad (\textbf{Schwarz inequality}) \tag{88}$$

We can understand this by looking at the simple 3D space analog where the *dot product* of two vectors is always smaller than or equal to the product of individual lengths of the vectors because of the cosine dependence of dot products.This fact can be used to set up an inequality which will result in the following statement:

Given two physical observable $A$ and $B$, the uncertainty in the measurement of the two is related to their *commutator*.

$$\boxed{\sigma_A^2\sigma_B^2 \geq \left(\frac{1}{2i}\left\langle[\hat{A},\hat{B}]\right\rangle\right)^2} \tag{89}$$

This is the **Generalized Uncertainty Principle**. For $\hat{A} = \hat{x}$ and $\hat{B} = \hat{p}$ along with postulate (4), we can get the famous position momentum uncertainty principle from eq(89)

$$\boxed{\sigma_x\sigma_y \geq \frac{\hbar}{2}} \tag{90}$$

We can find the rate of change of expectation value of any observable $A$ as follows:

$$\frac{d}{dt}\langle A\rangle = \frac{d}{dt}\langle\Psi|\hat{A}|\Psi\rangle = \left\langle\frac{\partial\Psi}{\partial t}\middle|\hat{A}\middle|\Psi\right\rangle + \langle\Psi|\left(\frac{\partial\hat{A}}{\partial t}\right)|\Psi\rangle + \left\langle\Psi\middle|\hat{A}\middle|\frac{\partial\Psi}{\partial t}\right\rangle$$

Using Schrodinger's equation to change the time derivatives of $|\Psi\rangle$, we get:

$$\boxed{\frac{d}{dt}\langle A\rangle = \frac{i}{\hbar}\left\langle[\hat{H},\hat{A}]\right\rangle + \left\langle\frac{\partial\hat{A}}{\partial t}\right\rangle} \tag{91}$$

This very important result, although not formally, but by many, is called **generalised Ehrenfest theorem**. It is also similar to eq(152). Note the implication that if operator associated with some observable *commutes* with the Hamiltonian, then that observable becomes a *constant of the motion* (Given that the operator did not have some explicit time dependence). For example, in case of a **free particle**, the Hamiltonian just consists a $\hat{p}^2$ term and hence Hamiltonian commutes with the momentum operator. Consequently, momentum of a free particle turns out to be a constant of the motion, a conserved quantity in time!

eq(91) also enables us to properly define Energy-Time uncertainty principle. If a quantity $A$ does NOT commute with the Hamiltonian and $A$ does not explicitly depend on time, we can use eq(89) and eq(91) together:

$$\sigma_H\sigma_A \geq \frac{\hbar}{2}\left|\frac{d\langle A\rangle}{dt}\right|$$

defining $\Delta E \equiv \sigma_H$ and

$$\Delta t \equiv \frac{\sigma_A}{|d\langle Q\rangle/dt|}$$

We can state the **Energy-Time uncertainty principle**:

$$\boxed{\Delta E \Delta t \geq \frac{\hbar}{2}} \tag{92}$$

$\Delta t$ can be interpreted as amount of time it takes the expectation value of $A$ to change by one standard deviation.

Next we state the **Virial Theorem** for stationary states. Let $T$ be the kinetic energy and $V$ be the potential energy , then

$$2\langle T\rangle = \left\langle x\frac{dV}{dx}\right\rangle \tag{93}$$

in three dimensions we have

$$\boxed{2\langle T\rangle = \langle \boldsymbol{r}\cdot\nabla V\rangle} \tag{94}$$

## 2.7 Angular Momentum

The operator associated with Angular momentum is motivated from the prescription in classical mechanics, i.e.,

$$\boldsymbol{L} = \boldsymbol{r}\times\boldsymbol{p}$$

Which gives

$$\hat{L_x} \equiv \hat{y}\hat{p_z} - \hat{z}\hat{p_y} \tag{95}$$

Similar forms for $\hat{L_y}$ and $\hat{L_z}$ are defined

$$\hat{L_y} \equiv \hat{z}\hat{p_x} - \hat{x}\hat{p_z} \quad \text{ and } \hat{L_z} \equiv \hat{x}\hat{p_y} - \hat{y}\hat{p_x} \tag{96}$$

The operators do not commute with each other, if fact

$$[L_x, L_y] = i\hbar L_z \quad ; [L_y, L_z] = i\hbar L_x \quad ; [L_z, L_x] = i\hbar L_y \tag{97}$$

So it is clear we cannot determine, for example, $L_x$ and $L_y$ simultaneously with infinite accuracy.

$$\sigma_{L_x}\sigma_{L_y} \geq \frac{\hbar}{2}|\langle L_z\rangle|$$

But the $L^2$ operator does commute with $L_x$ (and $L_y$, $L_z$).

$$L^2 \equiv L_x^2 + L_y^2 + L_z^2 \tag{98}$$

$$[L^2, \boldsymbol{L}] = 0 \tag{99}$$

So we find simultaneous eigenstates of (say) $L_z$ with $L^2$. This task is done in a similar way to what we did in the harmonic oscillator problem, we define two operators as follows:

$$L_\pm \equiv L_x \pm iL_y \tag{100}$$

After finding the commutators of these *ladder* operators with $L_z$ and $L^2$ we create an algebra which ultimately leads us to the result that

$$L^2 f_\ell^m = \hbar^2 \ell(\ell+1) f_\ell^m \quad ; L_z f_\ell^m = \hbar m f_\ell^m \tag{101}$$

where

$$\ell = 0, \frac{1}{2}, 1, \frac{3}{2}, ... \quad ; m = -\ell, -\ell+1, ..., \ell-1, \ell \tag{102}$$

Other than this, effect of lowering and raising operators is as follows:

$$L_+ f_\ell^m = \hbar\sqrt{\ell(\ell+1) - m(m+1)} f_\ell^{m+1} \tag{103}$$

$$L_- f_\ell^m = \hbar\sqrt{\ell(\ell+1) - m(m-1)} f_\ell^{m-1} \tag{104}$$

Furthermore, the rate of change of expectation value of the operator $\boldsymbol{L}$ is equal to expectation value of torque, i.e.,

$$\frac{d}{dt}\langle \boldsymbol{L} \rangle = \langle \boldsymbol{r} \times (-\nabla V) \rangle \tag{105}$$

For sperically symmetric potentials $V(\boldsymbol{r}) = V(r)$, we can show that

$$\frac{d}{dt}\langle \boldsymbol{L} \rangle = 0 \quad \textbf{(Conservation of Angular momentum)} \tag{106}$$

### 2.7.1 Spherical Harmonics

In spherical coordinate system, operator $\boldsymbol{L}$ turns out to be

$$\boldsymbol{L} = i\hbar \left( \hat{\phi}\frac{\partial}{\partial\theta} - \hat{\theta}\frac{1}{\sin\theta}\frac{\partial}{\partial\phi} \right) \tag{107}$$

Converting the unit vector back to Cartesian system we can find that

$$L_x = -i\hbar \left( -\sin\phi\frac{\partial}{\partial\theta} - \cos\phi\cot\theta\frac{\partial}{\partial\phi} \right) \tag{108}$$

$$L_y = -i\hbar \left( -\cos\phi\frac{\partial}{\partial\theta} - \sin\phi\cot\theta\frac{\partial}{\partial\phi} \right) \tag{109}$$

$$L_z = -i\hbar\frac{\partial}{\partial\phi} \tag{110}$$

These will help us define $L_\pm$ and hence we can find $L^2 f_\ell^m$ as

$$\left[ \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left( \sin\theta\frac{\partial}{\partial\theta} \right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2} \right] f_\ell^m = -\sqrt{\ell(\ell+1)} f_\ell^m \tag{111}$$

Solution to this equation are well known **Spherical harmonics**. Symbol used is $Y_\ell^m(\theta,\phi)$, it is a multiplication of some special polynomials and a term of form $e^{im\phi}$. It is defined as follows:

$$\boxed{Y_\ell^m(\theta,\phi) = \sqrt{\frac{(2\ell+1)}{4\pi}\frac{(\ell-m)!}{(\ell+m)!}} e^{im\phi} P_\ell^m(\cos(\theta))} \tag{112}$$

Where $P_\ell^m$ are **associated Legendre function** defined as

$$P_\ell^m(x) \equiv (-1)^m \left(1-x^2\right)^{m/2} \left(\frac{d}{dx}\right)^m P_\ell(x) \tag{113}$$

and $P_\ell(x)$ is the $\ell th$ **Legendre polynomial**, which is define by the **Rodrigues formula**:

$$P_\ell(x) \equiv \frac{1}{2^\ell \ell!} \left(\frac{d}{dx}\right)^\ell \left(x^2-1\right)^\ell \tag{114}$$

$P_\ell$ are orthogonal polynomials with

$$\int_{-1}^{1} P_\ell(x) P_{\ell'}(x) dx = \left(\frac{2}{2\ell+1}\right) \delta_{\ell\ell'} \tag{115}$$

## 2.8 Spin

Spin is another observable of quantum systems which manifests itself as some kind of angular momentum. Many say that the word spin itself is not a good description for this intrinsic fundamental property of quantum particles (Paul. M. Dirac preferred to call electron spin as "two valuedness"). Although it is hard to explain what is actually going on at that scale. Like a famous quote says: To understand electron spin, think of a ball spinning, but its not a ball and it is not spinning (Because if it were spinning, the speed of a point at the "equator" will be greater than the speed of light!). The mathematics of the theory of spin, on the other hand, is quite simple as compared to infinite dimensional linear algebra.
We start with *Postulating* the fundamental commutator relations which are motivated by the commutator relations of the angular momentum we discussed in eq(97). We denote the spin operator with the letter $S$. We have

$$[S_x, S_y] = i\hbar S_z \quad ;[S_y, S_z] = i\hbar S_x \quad ;[S_z, S_x] = i\hbar S_y \tag{116}$$

Both of these set of commutator relations follow the **rotational invariance** in 3D space. It follows that the eigenvetors of $S^2$ and $S_z$ satisfy

$$S^2 \left|s\ m\right\rangle = \hbar^2 s(s+1) S^2 \left|s\ m\right\rangle \tag{117}$$

$$S_z \left|s\ m\right\rangle = \hbar m \left|s\ m\right\rangle \tag{118}$$

$$S_\pm = \hbar\sqrt{s(s+1) - m(m\pm 1)} \left|s\ (m\pm 1)\right\rangle \tag{119}$$

where $S_\pm \equiv S_x \pm iS_y$. Here, $s$ and $m$ can take the following values

$$s = 0, \frac{1}{2}, 1, \frac{3}{2} \quad ; \quad m = -s, -s+1, ..., s-1, s$$

$s$ value for mesons is 0, for electrons it's 1/2, photons have spin 1, $\Delta$ baryons have spin 3/2, gravitons have spin 2, and so on.

### 2.8.1 Spin 1/2

For $s = 1/2$, there are just two eigenstates $\left|\frac{1}{2}\ \frac{1}{2}\right\rangle$ and $\left|\frac{1}{2}\ (-\frac{1}{2})\right\rangle$, these are also represented by $|\uparrow\rangle$ and $|\downarrow\rangle$ respectively. Using these states as basis vector, the general state of a spin-1/2 particle can be represented by a column matrix, it is also called a **spinor**.

$$\chi = \begin{pmatrix} a \\ b \end{pmatrix} = a\chi_+ + b\chi_-$$

In this basis the operator $\boldsymbol{S}$ can be found, and it turns out to be

$$\boldsymbol{S} = \frac{\hbar}{2}\boldsymbol{\sigma} \tag{120}$$

where

$$\boxed{\sigma_x \equiv \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; \quad \sigma_y \equiv \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}; \quad \sigma_z \equiv \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}} \tag{121}$$

These are **Pauli matrices**. While we are on this topic, we should mention that *any* 2×2 matrix $M$ can be expanded in terms of identity $I$ and these three Pauli matrices (Just like the natural basis in section 1.6). We may call them the Pauli basis.

$$M = \frac{\mathrm{Tr}(M)}{2}I + \alpha_1\sigma_x + \alpha_2\sigma_y + \alpha_3\sigma_z = \frac{\mathrm{Tr}(M)}{2}I + \boldsymbol{\alpha}\cdot\boldsymbol{\sigma}$$

Where $\alpha_i$ are weight constants that are easy to find by transforming the natural basis. Commutator relation is given by

$$[\sigma_k, \sigma_l] = 2i\epsilon_{klm}\sigma_m \tag{122}$$

An analytic form for exponential of a 2×2 matrix can be found using pauli basis:

$$e^M = e^{\frac{1}{2}\mathrm{Tr}(M)}\left(I\cosh(\alpha) + \frac{(\boldsymbol{\alpha}\cdot\boldsymbol{\sigma})}{\alpha}\sinh(\alpha)\right); \quad \text{where} \quad \alpha = \sqrt{\alpha_1 + \alpha_2 + \alpha_3} \tag{123}$$

Digression aside, eigenspinors of $\boldsymbol{S}$ are $\pm\frac{\hbar}{2}$. This helps us understand the results of the famous Stern-Gerlach experiment.

### 2.8.2 Larmor precession

A spinning charged particle constitutes a magnetic dipole with magnetic dipole moment $\boldsymbol{\mu}$ being proportional to the spin angular momentum $\boldsymbol{S}$:

$$\boldsymbol{\mu} = \gamma\boldsymbol{S}$$

where, $\gamma$ is called the **gyromagnetic ration**. In a magnetic field $\boldsymbol{B}$, a magnetic dipole will experience a torqu $\boldsymbol{\mu}\times\boldsymbol{B}$ , which tends to line it up parallel to the field. The energy associated with this torque is $-\boldsymbol{\mu}\cdot\boldsymbol{B}$. Hence the Hamiltonian is given by

$$H = -\gamma\boldsymbol{B}\cdot\boldsymbol{S} \tag{124}$$

If the magnetic field is a constant say $\boldsymbol{B} = B_0\hat{\boldsymbol{z}}$. Hamiltonian is just a $2 \times 2$ matrix given by

$$H = -\gamma B_0 S_z = -\frac{1}{2}\gamma B_0 \hbar \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{125}$$

Given some initial state $\chi$:

$$\chi = \begin{pmatrix} a \\ b \end{pmatrix}$$

We can find the expectation values of

$$\langle S_x \rangle = \frac{\hbar}{2}\sin(\alpha)\cos(\gamma B_0 t)$$

$$\langle S_y \rangle = -\frac{\hbar}{2}\sin(\alpha)\sin(\gamma B_0 t)$$

$$\langle S_z \rangle = \frac{\hbar}{2}\cos(\alpha)$$

where $a \equiv \cos(\alpha/2)$ and $b \equiv \sin(\alpha/2)$. Thus we can interpret that $\langle \boldsymbol{S} \rangle$ is tilted at a constant angle $\alpha$ to the z axis and precesses about the field at a **Larmor frequency**

$$\boxed{\omega = \gamma B_0} \tag{126}$$

### 2.8.3 Addition of Angular Momenta

If we have two particles with spins $s_1$ and $s_2$ in state $|s_1\ m_1\rangle$ and $|s_2\ m_2\rangle$ respectively. We denote the composite state by $|s_1 s_2\ m_1 m_2\rangle$. The total angular momentum is given by

$$|s\ m\rangle = \sum_{m_1+m_2=m} C^{s_1 s_2 s}_{m_1 m_2 m}\, |s_1 s_2\ m_1 m_2\rangle \tag{127}$$

where the constants $C^{s_1 s_2 s}_{m_1 m_2 m}$ are the **Clebsch-Gordan coefficient** and they are found by tensor products (or they can be copied from some table on the internet). Note that the z component $S_z$ is just the sum of m's, i.e., $m = m_1 + m_2$. For spin half particle , we get 4 composite states, that are :

$$|1\ 1\rangle = |\uparrow\uparrow\rangle$$

$$|1\ 0\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$$

$$|1\ -1\rangle = |\downarrow\downarrow\rangle$$

These are called the **triplet** combination with $s = 1$. Fourth one is called the **singlet** with $s = 0$

$$|0\ 0\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$$

## 2.9 Hamiltonian in electromagnetism

For classical electrodynamics, the Hamiltonian is defined as follows:

$$\boxed{\hat{H} = \frac{1}{2m}(\boldsymbol{p} - q\boldsymbol{A})^2 + q\varphi} \tag{128}$$

Here, $\boldsymbol{A}$ is called the vector potential which is associated with the magnetic fields, and $\varphi$ is the scalar potential associated with electric fields. There are defined as follows:

$$\boldsymbol{E} = -\nabla\varphi - \frac{\partial \boldsymbol{A}}{\partial t} \quad ; \quad \boldsymbol{B} = \nabla \times \boldsymbol{A} \tag{129}$$

Where $\boldsymbol{E}$ and $\boldsymbol{B}$ are , as usual, electric and magnetic fields. The Schrodinger equation (postulate 5) becomes

$$i\hbar\frac{\partial \Psi}{\partial t} = \left[\frac{1}{2m}(\boldsymbol{p} - q\boldsymbol{A})^2 + q\varphi\right]\Psi \tag{130}$$

The theory of electrodynamics is said to be **Gauge Invariant** as the electric or magnetic fields stay invariant under **gauge transformations**. For example, $\boldsymbol{B}$ is defined in eq(129) but since we have to take the *curl* of the vector potential $\boldsymbol{A}$, we can add any *gradient* of some scalar function to it and it will not change $\boldsymbol{B}$, i.e., if we define $\boldsymbol{A'}$ as

$$\boldsymbol{A'} \equiv \boldsymbol{A} + \nabla\chi \tag{131}$$

Now as curl of any gradient is zero,

$$\nabla \times \boldsymbol{A'} = \nabla \times (\boldsymbol{A} + \nabla\chi) = \nabla \times (\boldsymbol{A}) + \nabla \times (\nabla\chi) = \nabla \times \boldsymbol{A} + 0 = \nabla \times \boldsymbol{A} = \boldsymbol{B}$$

We may as well choose a gauge such that $\nabla \cdot \boldsymbol{A} = 0$. Such a gauge is called the **Coulomb Gauge**. Similarly, we can also change $\varphi$ as follows without changing the field $\boldsymbol{E}$

$$\varphi' \equiv \varphi - \frac{\partial\chi}{\partial t} \tag{132}$$

eq(131) and eq(132) are **gauge transformations**, where $\chi$ is related to the gauge. The effect of a gauge transformation on the wave function is to just add a *phase factor* to it, which gets cancelled out during taking the modulus square.

$$\Psi' = e^{iq\chi/\hbar}\Psi \tag{133}$$

## 2.10 The $1/|x|$ problem

Motivated by the fact that repulsion force between two electrons is of form $1/r^2$ and hence the potential is of form $1/r$, we try to solve a simple 1D scattering problem with a potential which is given by

$$V(x) = \frac{e^2}{4\pi\epsilon_0}\frac{1}{|x|} \tag{134}$$

Schrodinger equation becomes

$$\frac{\hbar^2}{2m_e}\frac{d^2\psi}{dx^2} + \frac{e^2}{4\pi\epsilon_0}\frac{1}{|x|}\psi = E\psi \tag{135}$$

where $e$ is the charge on electron and $m_e$ is its mass. It is a scattering problem and $E > 0$, we can define the following variables to simplify the equation

$$\kappa \equiv \frac{\sqrt{2m_e E}}{\hbar} \quad \text{(a positive constant)}; \quad \beta^2 \equiv \frac{e^2}{4\pi\epsilon_0}\frac{2m_e}{\hbar^2} \tag{136}$$

then eq(135) becomes

$$\frac{d^2\psi}{dx^2}\left(\kappa^2 - \frac{\beta^2}{|x|}\right)\psi = 0 \tag{137}$$

Solutions are given by a combination of complex exponential weighted by $x$ and **Confluent Hypergeometric functions**.

### 2.10.1 Confluent Hypergeometric functions

Confluent Hypergeometric functions are the solutions to the following differential equation

$$xy'' + [c - x]y' - ay = 0 \tag{138}$$

where $a$ and $c$ are constant parameters. Due to the presence of three regular singularities at $x = 0$, we use *Frobenius method* to solve this differential equation. Solutions are

$$M(a, c; x) = 1 + \frac{a}{c}\frac{x}{1!} + \frac{a(a+1)}{c(c+1)}\frac{z^2}{2!} + ... \quad \textbf{(Kummer's function)} \tag{139}$$

the other solution is

$$U(a, c; x) = \frac{\pi}{\sin \pi c}\left[\frac{M(a, c; x)}{\Gamma(a - c + 1)\Gamma(c)} - x^{1-c}\frac{M(a - c + 1, 2 - c; x)}{\Gamma(a)\Gamma(2 - c)}\right] \tag{140}$$

The second solution is called the **Tricomi's function**. Integral representation of Kummer's function is

$$M(a, c, x) = \frac{\Gamma(c)}{\Gamma(a)\Gamma(c - a)}\int_0^1 e^{tx}t^{a-1}(1 - t)^{c-a-1}dt \tag{141}$$

The solutions of eq(137) are

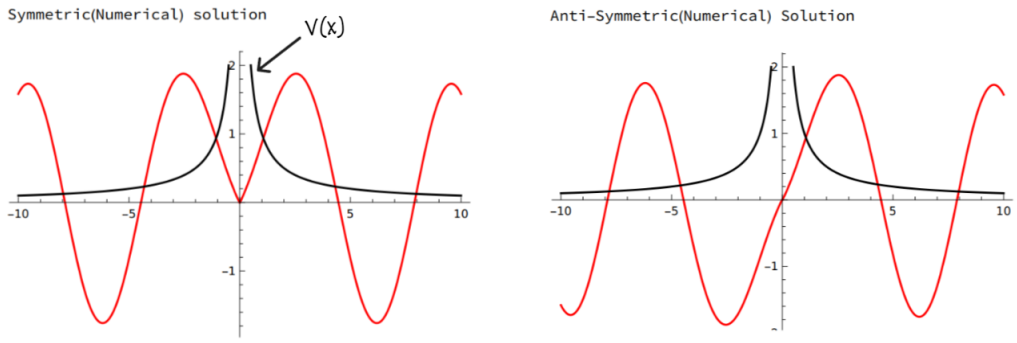
$$\psi(x) = \begin{cases} xe^{-i\kappa x}\left[a_1 M\left(1 - \frac{\beta^2}{2\kappa}i, 2; 2i\kappa x\right) + a_2 U\left(1 - \frac{\beta^2}{2\kappa}i, 2; 2i\kappa x\right)\right]; & x > 0 \\ xe^{-i\kappa x}\left[a_3 M\left(1 + \frac{\beta^2}{2\kappa}i, 2; 2i\kappa x\right) + a_4 U\left(1 + \frac{\beta^2}{2\kappa}i, 2; 2i\kappa x\right)\right]; & x < 0 \end{cases} \tag{142}$$

Here, $a_i$'s are constants that are fixed by boundary conditions: Continuity of wave function and discontinuity of wave function which is given by

$$\Delta\left(\frac{d\psi}{dx}\right) \equiv \lim_{\epsilon\to 0}\left(\left.\frac{\partial\psi}{\partial x}\right|_{+\epsilon} - \left.\frac{\partial\psi}{\partial x}\right|_{+\epsilon}\right) = \frac{2m}{\hbar^2}\lim_{\epsilon\to 0}\int_{-\epsilon}^{+\epsilon} V(x)\psi(x)dx \tag{143}$$

Note that if potential is not infinite (which is what happens practically), the integral on the right of eq(143) vanishes and hence derivative is continuous as well. But we are not

that lucky, because our problem *does* have a singularity at origin. Therefore, first derivative is discontinuous there.Furthermore, these states are not normalizable, though there linear combinations can give a function from $\mathcal{L}_2$. As the potential is symmetric, we can have either odd or even wave functions.The numerical solutions are plotted bellow:




# 3 Classical Mechanics

Here, we (very briefly) cover the two formalisms for classical mechanics, namely, Lagrangian and Hamiltonian mechanics. This will help us in semi-classical mechanics because many aspects of it are connected to ideas like the action, lagrangian, etc. This will also let us formalise the idea of the Hamiltonian we were using in the previous section.

## 3.1 The phase space

In modern dynamics we work in a phase space which was briefly discussed in the previous section. All the equations of motion can be turned into a system of first order differential equations, which can be solved either numerically or analytically. The idea is that every information about the position coordinates $q$ and velocity coordinates $\dot{q}$ is stored in the *components* of an abstract vector roaming around in a finite dimensional LVS called the **Phase space**. Given the initial vector, along with a time evolution rule, we can find the future.

## 3.2 Lagrangian formalism

The Lagrangian is often defined as the Kinetic minus the potential energy of a system:

$$\mathcal{L} \equiv T - V \tag{144}$$

This $\mathcal{L}$ is different than $\mathcal{L}_2$ space (we have just used the same symbol). The key insight in this method is a quantity called the **Action** $S$ is extremised on a trajectory that the classical particle "chooses". Action is defined as

$$S \equiv \int_{t_1}^{t_2} \mathcal{L}(q, \dot{q}, t) dt \tag{145}$$

We can also say that the first order change in $S$, i.e., $\delta S$ is 0. For generalised coordinates $(q_i, \dot{q}_i)$. The condition given in eq(148) leads to the **Euler-Lagrange equation** (or rather a set of equations for all $i$'s)

$$\frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{q}_i}\right) - \frac{\partial \mathcal{L}}{\partial q_i} = 0 \tag{146}$$

But Lagrangian may take different forms in other systems, it is not always $T - V$ as suggested in eq(144). For instance,if we look at the Lagrangian of a charged particle in an electomagnetic fields, it comes out to be:

$$\mathcal{L}(\boldsymbol{r}, \boldsymbol{v}, t) = \frac{1}{2}m\boldsymbol{v}^2 + q(\boldsymbol{A} \cdot \boldsymbol{v} - \phi) \tag{147}$$

Symbols were defined in eq(129).

### 3.2.1 Legendre Transforms

It is a transformation of variables. If we have a function $f(x)$ with a condition that $f'(x)$ is invertible, Then we can find a function $g(p)$ such that $f'(x)$ and $g'(x(p))$ are inverse functions of each other, i.e.,

$$f'(g'(x(p))) = \pm x = g'(f'(x)) \tag{148}$$

To transform we do the following

$$g = f - xp \tag{149}$$

This is a way of get rid of $x$ for $p$. This transformation from $f(x)$ to $g(p)$ is called the **Legendre Transform**

## 3.3 Hamiltonian formalism

When take the Legendre Transform of the Lagrangian in order to get rid of $\dot{q}$ from the denominators of partial derivatives (as we want work in position dependence rather than velocity dependence), we get the **Hamiltonian**:

$$H(q, p, t) \equiv \dot{q}p - \mathcal{L} \tag{150}$$

Combined with Euler-Lagrange equations we can find the **Hamilton's equations of motion**:

$$\dot{p}_i = -\frac{\partial H}{\partial q_i}; \quad \text{and } \dot{q}_i = \frac{\partial H}{\partial p_i} \tag{151}$$

If we have $N$ generalised coordinates then the phase space is $2N$ dimensional (unless we give time its own axis, then it is $2N + 1$ dimensional).

**Poisson brackets** of two objects $A$ and $B$ in this formalism is a short hand for:

$$\{A, B\} = \sum_i \left(\frac{\partial A}{\partial q_i}\frac{\partial B}{\partial p_i} - \frac{\partial B}{\partial q_i}\frac{\partial A}{\partial p_i}\right)$$

and the corresponding canonical commutation relations are

$$\{q_i, p_j\} = \delta_{ij}$$

$$\{q_i, q_j\} = \{p_i, p_j\} = 0$$

It turns out, time evolution of some quantity $F$ is related to the poisson brackets as follows:

$$\frac{dF}{dt} = \{F, H\} + \frac{\partial F}{\partial t} \tag{152}$$

If the right hand side is 0, then $F$ and $H$ are said to be in **involution** with each other. We can see that eq(153) is similar to the quantum analog eq(91).

If we have set of dynamical equations:

$$\dot{x}_1 = f_1(x_1, x_2, ..., x_n)$$

$$.$$

$$.$$

$$\dot{x}_n = f_n(x_1, x_2, ..., x_n)$$

We can clump them by defining q vector $\boldsymbol{x} \equiv (x_1, x_2, ..., x_n)$. Using the Hamilton's equations of motion, we can write the time evolution of $\boldsymbol{x}$:

$$\boxed{\dot{\boldsymbol{x}} = J\nabla H} \tag{153}$$

where, $J$ is a $2n \times 2n$ matrix:

$$J \equiv \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} \tag{154}$$

and the operator $J\nabla$ is called the **Symplectic gradient**. Furthermore, we may write the poisson bracket in the Symplectic space :

$$\{A, B\} = (\nabla A)^T J(\nabla B) \quad \textbf{(Symplectic Dot product)} \tag{155}$$

If this poisson bracket turns out to be zero, $A$ and $B$ are (as expected) Symplectic orthogonal

# 4 Semi-Classical Mechanics

I have not covered a few topics in the section on quantum mechanics because there was some overlap between them and this section on Semi Classical mechanics, another reason was balancing the lengths of the sections.

## 4.1 Classical limit

### 4.1.1 Probability Current Density

We start by defining the **Probability Current density**. Recalling the equation that governs the conservation of charge in classical electrodynamics:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \boldsymbol{j} = 0 \tag{156}$$

where $\boldsymbol{j}$ is the volume current density. A similar relation ship is found in quantum mechanics where $\rho$ replaces the probability density $|\Psi|^2$ and $\boldsymbol{j}$ is replaced by the following

$$\boldsymbol{j} \equiv \frac{i\hbar}{2m}(\Psi\nabla\Psi^* - \Psi^*\nabla\Psi) \tag{157}$$

giving a similar result

$$\boxed{\frac{\partial}{\partial t}|\Psi|^2 + \nabla \cdot \boldsymbol{j} = 0} \tag{158}$$

Although, the potential is considered to be *real* here. If potential has a non real part then probability is not conserved in time (this is used in particle physics to accommodate the absorption of elementary particles).

### 4.1.2 Hamilton-Jacobi equation

If we consider the following form on the wave function:

$$\Psi(\boldsymbol{r}, t) = \sqrt{\rho(\boldsymbol{r}, t)}\exp\left(\frac{iS(\boldsymbol{r}, t)}{\hbar}\right) \tag{159}$$

Were $\rho$ stands for $|\Psi|^2$ as discussed. Then substituting this form in the Schrodinger's equation (66), and assuming that $\hbar \to 0$ we get the following equation:

$$\boxed{\frac{1}{2m}|\nabla S(\boldsymbol{r}, t)|^2 + V(\boldsymbol{r}) + \frac{\partial S(\boldsymbol{r}, t)}{\partial t} = 0} \tag{160}$$

But this is the **Hamilton-Jacobi equation** from classical mechanics. So we say that as $\hbar \to 0$ quantum mechanics approaches classical mechanics. Furthermore, it lets us interpret the "quantity Phase times $\hbar$" as the **Action** or **Hamilton's Principle Function** in quantum mechanics.

## 4.2 Density operators

### 4.2.1 Pure States

The state vector $|\Psi\rangle$ is called a pure state. Although, the theory in *inherently* probabilistic, but if we know the state of a system, we can find expectation value of any observable $A$:

$$\langle A\rangle = \langle\Psi|\hat{A}|\Psi\rangle \tag{161}$$

In this sense we "know" everything about the system. But in practice, we are ignorant of even that. We formulate the theory in the following way:
We define a *density operator* $\hat{\rho}$:

$$\hat{\rho} \equiv |\Psi\rangle\langle\Psi| \tag{162}$$

In case this operator is given by a *matrix* (like in case of Spin), we can find its $ij$ element (With respect to an orthonormal basis $|e_j\rangle$):

$$\rho_{ij} = \langle e_i|\hat{\rho}|e_j\rangle \tag{163}$$

Then the expectation value of the observable $A$ is given by the *Trace* of this **density matrix** times the matrix $\hat{A}$:

$$\langle A \rangle = \mathrm{Tr}\Big(\rho \hat{A}\Big) \tag{164}$$

Other than that, $\rho$ is hermitian, its trace is unity and it is *idempotent*

$$\mathrm{Tr}(\rho) = 1 \tag{165}$$

$$\rho^\dagger = \rho \quad ; \rho^2 = \rho \tag{166}$$

### 4.2.2 Mixed States

When we do not know the state of the particle we say that the particle is in a mixed state. If we say that the probabilty of particle being in a state $|\Psi_k\rangle$ is $p_k$, then we can define the density operator as follows

$$\boxed{\hat{\rho} \equiv \sum_k p_k \left|\Psi_k\right\rangle \left\langle\Psi_k\right|} \tag{167}$$

Turns out most properties that were discussed in the case of pure states hold even in the mixed states, i.e.,

$$\rho^\dagger = \rho \quad \textbf{(Hermiticity)}$$

$$\mathrm{Tr}(\rho) = 1$$

$$\langle A \rangle = \mathrm{Tr}\Big(\rho \hat{A}\Big)$$

It is NOT idempotent though

$$\rho^2 \neq \rho \quad \text{Hence} \quad \mathrm{Tr}\big(\rho^2\big) \neq 1$$

Thus the quantity $\mathrm{Tr}\big(\rho^2\big)$ also gives a a measure of *purity*.

Time evolution of the density operator is given by

$$\boxed{i\hbar \frac{d\hat{\rho}}{dt} = [\hat{H}, \hat{\rho}]} \tag{168}$$

eq(137) holds when $dp_k/dt = 0$ for all $k$. Note that this equation is the classical analog of the Liouville equation,

$$\frac{\partial \rho_{cl}}{\partial t} = \{H_{cl}, \rho_{cl}\}$$

where $\{,\}$ represents poisson bracket. eq(169) is called **Liouville-von Neumann equation**

## 4.3 Wigner Distribution

Given a wave packet $\Psi(x)$, we define the Wigner distribution function, $f_W(p,q)$, as

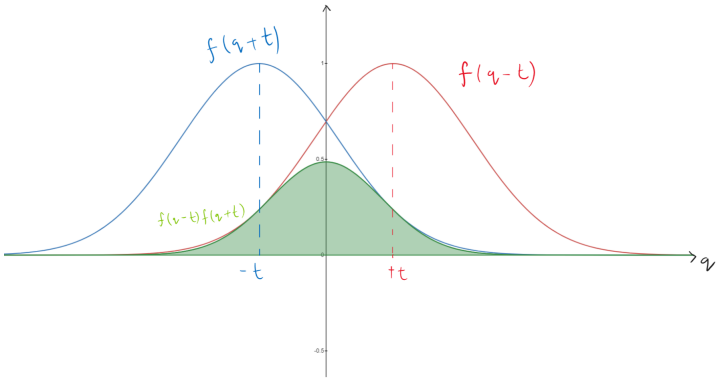
$$\boxed{f_W(p,q) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} e^{ips/\hbar} \left\langle q - \frac{s}{2} \middle| \Psi \right\rangle \left\langle \Psi \middle| q + \frac{s}{2} \right\rangle ds} \tag{169}$$

But

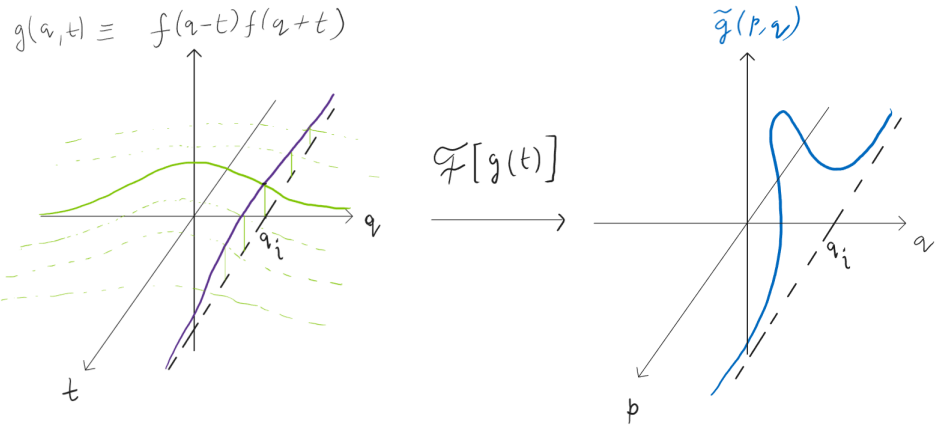
$$\left\langle q - \frac{s}{2} \middle| \Psi \right\rangle = \Psi\left(q - \frac{s}{2}\right)$$

$$\left\langle \Psi \middle| q + \frac{s}{2} \right\rangle = \Psi^* \left( q + \frac{s}{2} \right)$$

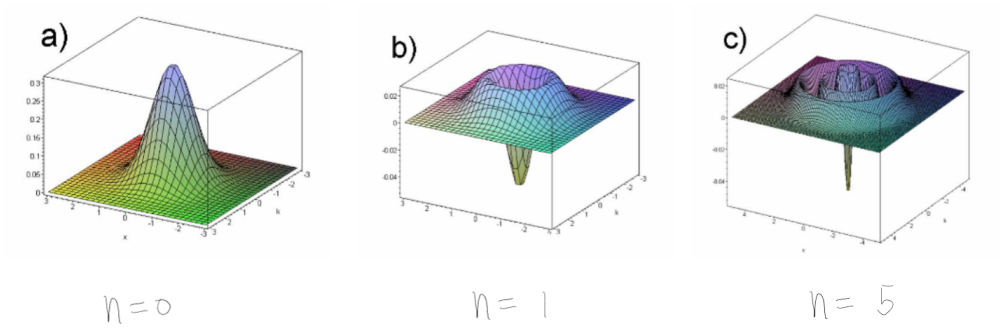
To visualise this a bit we may think of the following scenario. For some function $f(q)$ finding $f(q-t)$ is like shifting the whole function graph to the right by an amount $t$ (for $f(q+t)$ it is like shifting to left). We may think of $t = s/2$ if we like. Looking at the area under $t$ vs $f(q-t)f(q+t)$ is like quantifying the amount of overlap.




We can call the function $f(q-t)f(q+t)$ an overlap function (Note that the shape of the wave packet is fixed by $f(q)$ we are only looking at *shifts* in $f(q)$). Then fix some $q$ (lets call it $q_i$) and see the effect of varying $t$ *at this* $q_i$ this will give us a function that varies with $t$, i.e., $g_{q_i}(t)$, take the Fourier Transform of this function $g$ to bring it to $p$ domain from $t$ domain which gives us something like $\tilde{g}_q(p)$ (in the diagram since the overlap function ). We repeat this process for all different $q_i$'s and generate a two dimensional function $\tilde{g}_W(p,q)$. This is our distribution function.




This distribution is a **Quasi-Probability Distribution** because it can take negative values, so it is not a *true* probability distribution. Below is an example of Wigner distributions for some energy eigenstates of quantum harmonic oscillator (labelled by $n$).




We may also write this distribution in terms of density operator:

$$f_W(p,q) = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} e^{ips/\hbar}\left\langle q - \frac{s}{2}\middle|\hat{\rho}\middle|q + \frac{s}{2}\right\rangle ds \tag{170}$$

Equation of motion for this distribution can be found by considering eq(169) and taking the wigner transform on both sides, giving us

$$\frac{\partial \rho_W}{\partial t} = H_W \exp\left(-\frac{i\hbar}{2}\Lambda\right)\rho_W - H_W \exp\left(\frac{i\hbar}{2}\Lambda\right)\rho_W \tag{171}$$

Where $\Lambda$ stands for poisson bracket. Hence we get the time evolution of Wigner Distribution:

$$\boxed{\rho_W(t) = \exp\left(-\frac{2t}{\hbar}H_W \sin\left(\frac{\hbar}{2}\Lambda\right)\right)\rho(0)} \tag{172}$$

We can see for the lowers order in $\hbar$ we get

$$\frac{d\rho_W}{dt} = -H_W \Lambda \rho_W = \{H_W, \rho_W\}$$

which is just eq(137). Furthermore, given the Wigner distribution, we can find $|\Psi(q)|^2$ and $|\tilde{\Psi}(p)|^2$ as follows:

$$\int_{-\infty}^{\infty} f_W(p,q)dp = \langle q|\Psi\rangle\langle\Psi|q\rangle = |\Psi(q)|^2$$

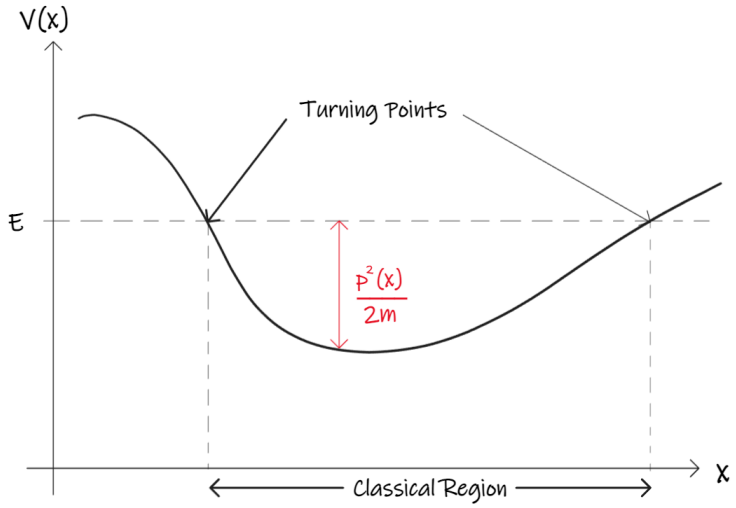
$$\int_{-\infty}^{\infty} f_W(p,q)dq = \langle p|\Psi\rangle\langle\Psi|p\rangle = |\tilde{\Psi}(p)|^2$$

Also

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} f_W(p,q)\ \ dp\ \ dq = 1$$

## 4.4 WKB approximation

The WKB (Wentzel, Kramers, Brillouin) method is a technique for obtaining approximate solutions to time-independent Schrodinger equation. It is also useful in calculating bound state energies and tunneling rates through potential barriers.




We define $p(x)$ for some potential $V(x)$ as follows

$$p(x) \equiv \sqrt{2m[E - V(x)]} \tag{173}$$

then the Schrodinger equation becomes

$$\frac{d^2\psi}{dx^2} = -\frac{p^2}{\hbar^2}\psi \tag{174}$$

We let $E > V(x)$ for the moment (the classical region). Assuming the solution of kind

$$\psi(x) = A(x)e^{i\phi(x)} \tag{175}$$

and substituting in eq(155), we get the following equations (by separating the real and imaginary parts)

$$A'' = A\left[(\phi')^2 - \frac{p^2}{\hbar^2}\right]; \quad \left(A^2\phi'\right)' = 0 \tag{176}$$

For solving the first one we assume that $A''/A$ is much less than both $(\phi')^2$ and $p^2/\hbar^2$. This is the part where we enter into WKB approximation regime.

$$\phi(x) = \pm\frac{1}{\hbar}\int p(x)dx \quad \text{and} \quad A = \frac{C}{\sqrt{p(x)}} \tag{177}$$

hence the approximate solution becomes

$$\boxed{\psi(x) \approx \frac{C}{\sqrt{p(x)}} \exp\left(\pm\frac{i}{\hbar}\int p(x)dx\right)} \tag{178}$$

For non-classical regions

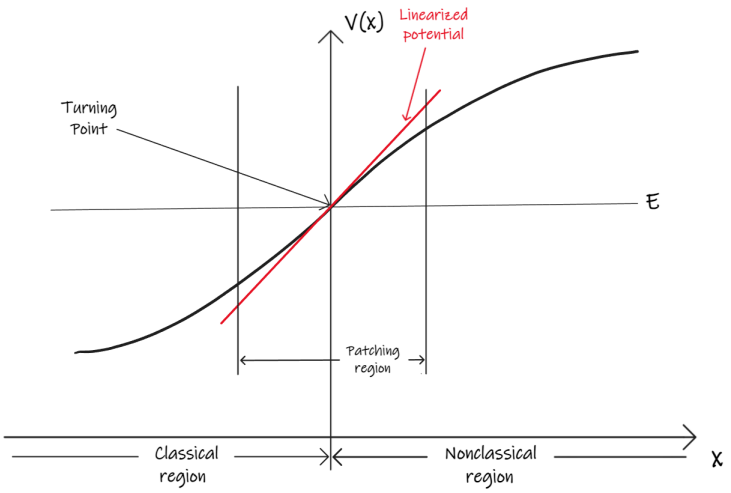
### 4.4.1 Airy functions

Near the classical turning points, $E \to V(x)$ and hence $p(x) \to 0$. Therefore the solutions given by eq(179) will not work because denominator goes to zero. We approximate the solutions near the turning points by **Airy functions**. Idea is to replace the potential at the turning point by it first order Taylor approximation, i.e, a linear approximation

$$V(x) \approx E + V'(0)x \tag{179}$$

Now we try to solve for the wave function $\psi_p$ in the patching region (see figure below).Defining $\alpha$ and $z$ such that

$$\alpha \equiv \left(\frac{2m}{\hbar^2}V'(0)\right)^{1/3}; \quad z \equiv \alpha x \tag{180}$$




We can write the Schrodinger equation as

$$\frac{d^2\psi_p}{dx^2} = z\psi_p \tag{181}$$

This is **Airy's equation** and the solutions are **Airy functions**:

$$\boxed{\psi_p(x) = a\mathrm{Ai}(\alpha x) + b\mathrm{Bi}(\alpha x)} \tag{182}$$

Airy functions can be represented in integral form as follow

$$\mathrm{Ai}(z) = \frac{1}{\pi}\int_0^\infty \cos\left(\frac{s^3}{3} + sz\right) ds \tag{183}$$

$$\mathrm{Bi}(z) = \frac{1}{\pi}\int_0^\infty \left[\exp\left(-\frac{s^3}{3} + sz\right) + \sin\left(\frac{s^3}{3} + sz\right)\right] ds \tag{184}$$

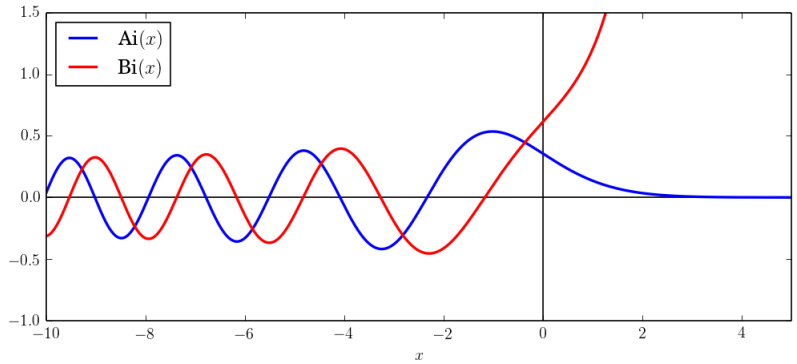
Their *Asymptotic forms* for $z >> 0$ is:

$$\mathrm{Ai}(z) \sim \frac{1}{2\sqrt{\pi}z^{1/4}}e^{-\frac{2}{3}z^{3/2}}; \quad \mathrm{Bi}(z) \sim \frac{1}{\sqrt{\pi}z^{1/4}}e^{\frac{2}{3}z^{3/2}}; \tag{185}$$

for $z << 0$:

$$\text{Ai}(z) \sim \frac{1}{\sqrt{\pi}(-z)^{1/4}} \sin\left[\frac{2}{3}(-z)^{3/2} + \frac{\pi}{4}\right]; \quad \text{Bi}(z) \sim \frac{1}{\sqrt{\pi}(-z)^{1/4}} \cos\left[\frac{2}{3}(-z)^{3/2} + \frac{\pi}{4}\right] \tag{186}$$

Here is how they look:

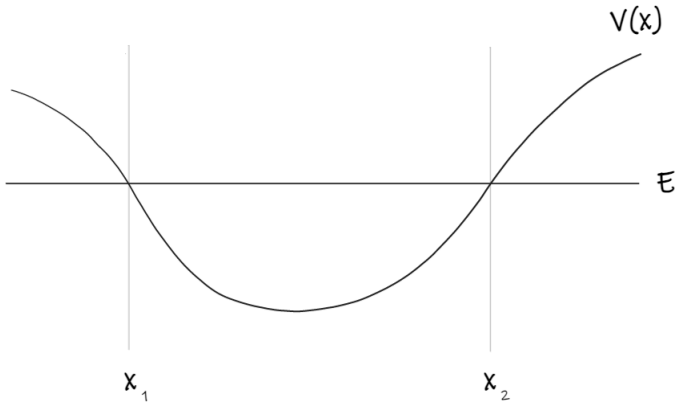



We can now find the expressions $\psi$ in general (in terms of on normalization constant $D$). We may also shift the turning point to some point $x_2$.

$$\psi(x) \approx \begin{cases} \frac{2D}{\sqrt{p(x)}} \sin\left[\frac{1}{\hbar}\int_x^{x_2} p(x')dx' + \frac{\pi}{4}\right], & x < x_2; \\ \frac{D}{\sqrt{|p(x)|}} \exp\left[-\frac{1}{\hbar}\int_{x_2}^{x} |p(x')|dx'\right], & x > x_2; \end{cases} \tag{187}$$

### 4.4.2 Bound state energies

For some potential well bounded between $x_1$ and $x_2$:




We can write the wave function in the interior region using eq(188) as

$$\psi(x) \approx \frac{2D}{\sqrt{p(x)}} \sin\left[\frac{1}{\hbar}\int_x^{x_2} p(x')dx' + \frac{\pi}{4}\right] \tag{188}$$

But we could have done the whole derivation in section 3.4.1 using a slope pointing 'downwards', that would have given us the wave function in that same region $x > x_1$ as

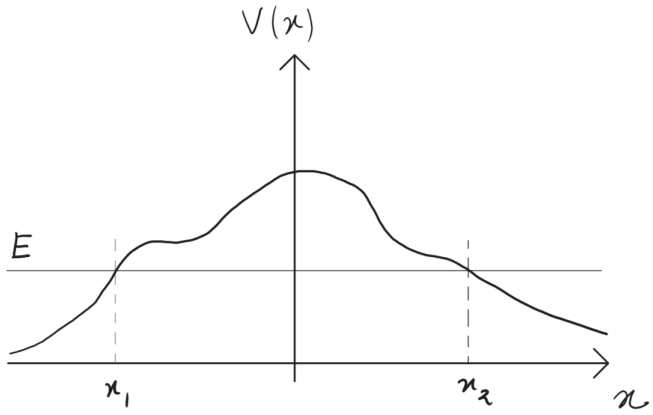
$$\psi(x) \approx \frac{-2D'}{\sqrt{p(x)}} \sin\left[-\frac{1}{\hbar}\int_{x_1}^{x} p(x')dx' - \frac{\pi}{4}\right] \tag{189}$$

This means that arguments of sine functions must differ by some multiple of $\pi$ hence we get

$$\boxed{\int_{x_1}^{x_2} p(x)dx = \left(n - \frac{1}{2}\right)\pi\hbar} \quad \text{with} \quad n = 1, 2, 3, ... \tag{190}$$

This quantization condition determines the allowed energies for a potential well. In semi-classical regime (large $n$), this result works quite well. Further more, it is easy to check that eq(191) gives the exact result for energy quantization in the case of harmonic oscillator, $V(x) = m\omega^2 x^2/2$

### 4.4.3 Tunneling




For tunneling probabilities in potential hills we get the following result:

$$T \sim e^{-2\gamma} \quad \text{where} \quad \gamma \equiv \frac{1}{\hbar}\int_{x_1}^{x_2} |p(x)|dx \tag{191}$$

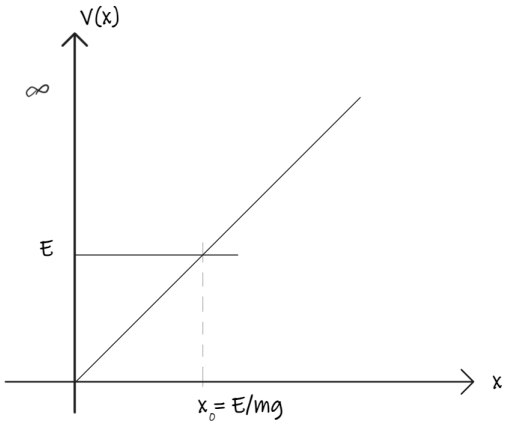
and wave function after proper connections become

$$\psi(x) \approx \begin{cases} \frac{1}{\sqrt{p(x)}}\left[Ae^{-\frac{i}{\hbar}\int_x^{x_1} p(x')dx'} + Be^{\frac{i}{\hbar}\int_x^{x_1} p(x')dx'}\right], & x < x_1; \\ \frac{1}{\sqrt{|p(x)|}}\left[Ce^{\frac{1}{\hbar}\int_{x_1}^{x} |p(x')|dx'} + De^{-\frac{1}{\hbar}\int_{x_1}^{x} |p(x')|dx'}\right], & x_1 < x < x_2; \\ \frac{1}{\sqrt{p(x)}}\left[Fe^{\frac{i}{\hbar}\int_{x_2}^{x} p(x')dx'}\right], & x > x_2; \end{cases} \tag{192}$$

### 4.4.4 The Bouncing ball problem

We model a potential for a bouncing ball:

$$V(x) = \begin{cases} mgx, & x > 0; \\ \infty, & x \leq 0. \end{cases} \tag{193}$$




as the potential is just linear on the right side, the solutions are exactly the Airy functions, although they are shifted by an amount determined by the energy $E$. Schrodinger equation reads (for $x \geq 0$)

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + mgx\psi = E\psi \tag{194}$$

We can simplify the above equation by introducing

$$z \equiv ax \quad \text{where} \quad a \equiv \left(\frac{2m^2 g}{\hbar^2}\right)^{1/3} \tag{195}$$

and

$$\epsilon \equiv \left(\frac{2}{m\hbar^2 g^2}\right)^{1/3} E \tag{196}$$

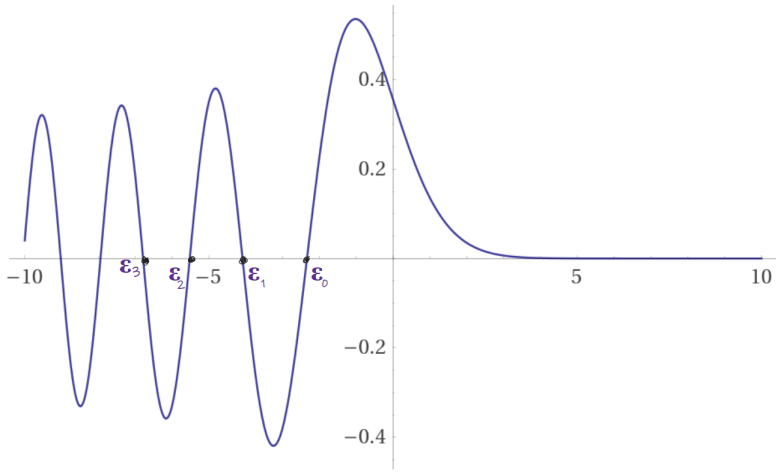
We also define $y(z) \equiv (1/\sqrt{a}\psi(x))$. Then the equation reads

$$y''(z) = (z - \epsilon)y(z) \tag{197}$$

This is just the Airy's equation eq(182) with inputs *shifted* by an amount $\epsilon$. Consequently, the solutions are

$$\psi(x) = D\mathrm{Ai}(ax - \epsilon) \tag{198}$$

We have not considered the solutions Bi because they blow up as $x \to \infty$. Now we can also use the fact that $\psi(0) = 0$ as a boundary condition to find the allowed energy values or $\epsilon$, which is just a root finding problem. For example, we see in the figure below that the function Ai(x) has infinite nodes of the left side. To find the $n$th energy eigenfunction and eigenvalue we just find the $n$th root of Ai(x) ($n$ =0, 1, 2, 3, ..). That gives us $\epsilon_n$.



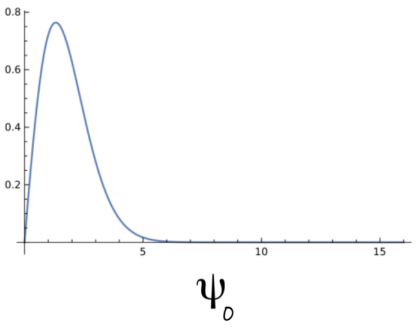

Then the energy eigen function is

$$\boxed{\psi_n(x) = D_n \mathrm{Ai}(ax - \epsilon_n)} \tag{199}$$

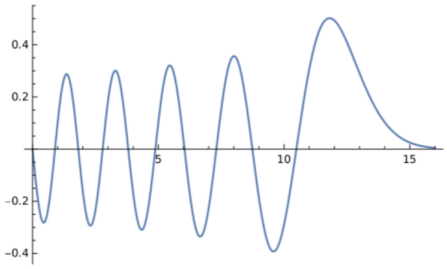
That is we just shift the graph of Ai(x) towards right such that the $n$th node is at origin. $D_n$ is the normalisation constant which we evaluate numerically. Energy is given by

$$\boxed{E_n = \left(\frac{m\hbar^2 g^2}{2}\right)^{1/3} \epsilon_n} \tag{200}$$

The ground state and the 10th energy eigen state are plotted below




$\psi_0$

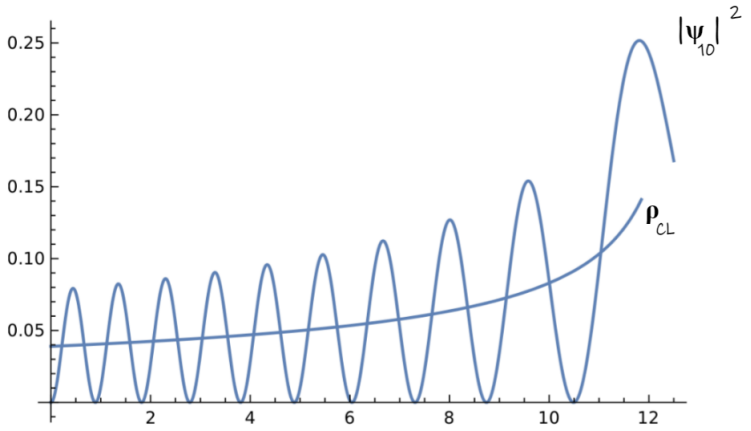



$\psi_{10}$

Classically, the probability goes like

$$\rho_{CL} = \frac{mg}{2\sqrt{E(E - mgx)}}; \quad \text{which in our units is} \quad \rho_{CL} = \frac{1}{\sqrt{\epsilon(\epsilon - x)}} \tag{201}$$

Comparing the plots of classical probability distribution and quantum one for a large $n$ such as $n = 10$. We see the match up, confirming our results




We can also find the allowed energies using WKB method using eq(191). Defining $x_0 \equiv E/mg$ (see figure below eq(194)).

$$\int_0^{x_0} \sqrt{2m(E-mgx)}dx = \left(n - \frac{1}{4}\right)\pi\hbar \tag{202}$$

For potentials closed off by $\infty$ at one side we use the factor $(n-1/4)$ and for potentials closed off on both sides (like particle in a box), we just use $n$ (or $n-0$ if you like). Doing the integral (or looking it up on wolfram) we get

$$\boxed{E_n = \left[\frac{9}{8}\pi^2 m g^2 \hbar^2 \left(n - \frac{1}{4}\right)^2\right]^{1/3}} \quad \textbf{(WKB approximation)} \tag{203}$$

Using eq(181) and eq(184) to compare the energies (for the sake of convenience, we use $g = 9.8m/s^2$ and mass of 100 grams) , we get energies of first four states as follow:

| $n$ | $\text{Energy}_{\text{exact}}$(J) | $\text{Energy}_{\text{WKB}}$ (J) | % Error |
|---|---|---|---|
| 0 | $8.81 \times 10^{-23}$ | $8.74 \times 10^{-23}$ | 0.794 |
| 1 | $1.54 \times 10^{-22}$ | $1.54 \times 10^{-22}$ | 0 |
| 2 | $2.08 \times 10^{-22}$ | $2.08 \times 10^{-22}$ | 0 |
| 3 | $2.56 \times 10^{-22}$ | $2.56 \times 10^{-22}$ | 0 |

Energy levels found by WKB method agrees precisely to 3 significant digits (except for ground state $n = 0$).

## 4.5 Path Integral Formulation

This formulation of quantum mechanics was given by Richard Feynman. In classical Lagrangian mechanics, the trajectory on which the action is extremum is chosen by the particle. According to this formulation, the probability amplitude of finding a particle at a position

$x'$ at some time $t'$ given that it was at $x_0$ at time $t_0$ initially is given by the summing a quantity related the *action* of the particle over ALL the possible paths it could take.

$$\langle x', t'|x_0, t_0\rangle = \int_{x_0}^{x'} D[x(t)] \exp\left(\frac{i}{\hbar} S[x(t)]\right) \tag{204}$$

where $S$ is the action given by

$$S[x(t)] = \int_{t_0}^{t'} dt L(x, \dot{x}) \tag{205}$$

and

$$\int_{x_0}^{x'} D[x(t)] \equiv \lim_{N\to\infty} \int_{-\infty}^{\infty} dx_1 .. \int_{-\infty}^{\infty} dx_{N-1} \left(\frac{m}{i2\pi\hbar\Delta t}\right)^{N/2} \tag{206}$$

eq(205) is known as **Feynman's Path integral**. In the limit $h \to 0$, i.e., in classical mechanics, the contributions from the paths that are different from extremum tend to vanish as the exponential in eq(205) oscillates more violently. So the contributions from the extremum path survives hence classical particle chooses the trajectory of extreme action.

## 4.6 Propagators

Propagators govern the time evolution of the state of the system. They are unitary because the norm (or probability) of the state vector should be preserved. We start with the fact that

$$|\Psi(t)\rangle = \exp\left[\frac{-i}{\hbar} H(t - t_0)\right] |\Psi(t_0)\rangle$$

inserting a complete set $a'$ we get

$$|\Psi(t)\rangle = \sum_{a'} |a'\rangle \langle a'|\Psi(t_0)\rangle \exp\left[\frac{-i}{\hbar} E_{a'}(t - t_0)\right]$$

in position basis $\boldsymbol{x'}$ we get

$$\psi(\boldsymbol{x'}, t) = \sum_{a'} c_{a'}(t_o) u_{a'} \exp\left[\frac{-i}{\hbar} E_{a'}(t - t_0)\right]$$

with

$$u_{a'} = \langle \boldsymbol{x'}|a'\rangle$$

standing for eigenfunctions of operator $A$ with eigenvalue $a'$, and $c_{a'}(t_0)$'s are given by

$$c_{a'}(t_0) = \int d^3x' u^*_{a'} \psi(\boldsymbol{x'}, t_0)$$

Hence we may write

$$\psi(\boldsymbol{x''}, t) = \int d^3x' K(\boldsymbol{x''}, t; \boldsymbol{x'}, t_o) \psi(\boldsymbol{x'}, t_0) \tag{207}$$

Where the kernel of the integral operator is known as the **propagator**. Here it is given by,

$$K(\boldsymbol{x''}, t; \boldsymbol{x'}, t_o) = \sum_{a'} |a'\rangle \langle \boldsymbol{x''}|a'\rangle \langle a'|\boldsymbol{x'}\rangle \exp\left[\frac{-i}{\hbar} E_{a'}(t - t_0)\right] \tag{208}$$

### 4.6.1 Van Vleck Propagator

The action $S$ can be expanded in terms of various orders of $\delta q$:

$$S = S_0 + \delta S_0 + \frac{1}{2}\delta^2 S_0 + ... \tag{209}$$

The third term is the second variation of $S$ around the classical trajectory which can be written explicitly as

$$\delta^2 S_0 = \int_{t'}^{t''} \delta q(t) \left\{ -V''(q_0(t)) - m\frac{d^2}{dt^2} \right\}$$

If we expand $\delta q(t)$ in a basis of orthogonal eigenfunctions of operator $\Lambda$:

$$\Lambda \equiv -V''(q_0(t)) - m\frac{d^2}{dt^2}$$

That is, we define a set of basis functions in time, $\{u_n(t)\}$:

$$\Lambda u_n(t) = \lambda_n u_n(t); \quad u_n(t') = u_n(t'') = 0 \tag{210}$$

then

$$\delta q(t) = \sum_n a_n u_n(t)$$

and

$$\delta^2 S = \sum_n \lambda_n a_n^2 \tag{211}$$

The path integral defined in equation (205) can also be written as

$$\langle x'|e^{-iHt/\hbar}|x\rangle = \lim_{N\to\infty} \left(\frac{m}{i2\pi\hbar t}\right) \int e^{iS(x,x',t)/\hbar} \prod_{n=1}^{N} da_n \left(\frac{\lambda_n^{(0)}}{2\pi i\hbar}\right)^{1/2} \tag{212}$$

replacing the $S$ in path integral by a term up to second order, replacing $\delta^2 S$ using eq(212), we can get a semi-classical approximation of the path integral, i.e,

$$\boxed{\langle \boldsymbol{x'}|e^{-iHt/\hbar}|\boldsymbol{x}\rangle^{SC} = \sum_{\text{all classical paths}} \left(\frac{1}{2\pi i\hbar}\right)^{n/2} \left[\det\left(\frac{-\partial^2 S}{\partial \boldsymbol{x'}\partial \boldsymbol{x}}\right)\right]^{1/2}} \tag{213}$$

This is called the **van Vleck propagator**.

### 4.6.2 Herman Kluk Propagator

In this scheme, for propagating wavepackets semi-classically, we first decompose the initial wavepacket into a set of coherent states. Coherent states maybe chosen such that their centers form an evenly spaced grid in the phase space. Then we propagate these coherent states, letting their centers move in time according to the classical mechanics. The width is kept fixed at initial value, hence these are also called *frozen gaussians*. The central classical trajectory is called the *guiding trajectory*. Then, we take the phase of the wavepacket to be

the classical action integral along the path of the guiding trajectory. The expression for the semiclassical propagator derived by Herman and Kluk in $N$ dimensions takes the form

$$\boxed{K(\boldsymbol{x''},t;\boldsymbol{x'},0)=\frac{1}{(2\pi\hbar)^N}\int\int d\boldsymbol{p'}d\boldsymbol{q'}R_{\boldsymbol{p'q'}t}e^{iS(\boldsymbol{p'q'}t)/\hbar}g_\gamma(\boldsymbol{q_t},\boldsymbol{p_t},\boldsymbol{x''})g^*_\gamma(\boldsymbol{q'},\boldsymbol{p'},\boldsymbol{x'})} \quad (214)$$

where

$$g_\gamma(\boldsymbol{q'},\boldsymbol{p'},\boldsymbol{x'})=\left(\frac{\gamma}{\pi}\right)^{N/4}\exp\left(-\frac{\gamma}{2}(\boldsymbol{x'}-\boldsymbol{q'})^2+\frac{i}{\hbar}\boldsymbol{p'}(\boldsymbol{x'}-\boldsymbol{q'})\right) \quad (215)$$

$$g_\gamma(\boldsymbol{q_t},\boldsymbol{p_t},\boldsymbol{x''})=\left(\frac{\gamma}{\pi}\right)^{N/4}\exp\left(-\frac{\gamma}{2}(\boldsymbol{x''}-\boldsymbol{q_t})^2+\frac{i}{\hbar}\boldsymbol{p_t}(\boldsymbol{x''}-\boldsymbol{q_t})\right) \quad (216)$$

and

$$R_{\boldsymbol{p'q'}t}=\sqrt{\det\left(\frac{1}{2}\left(\frac{\partial\boldsymbol{p_t}}{\partial\boldsymbol{p'}}+\frac{\partial\boldsymbol{q_t}}{\partial\boldsymbol{q'}}-i\gamma\hbar\frac{\partial\boldsymbol{q_t}}{\partial\boldsymbol{p'}}+\frac{i}{\hbar\gamma}\frac{\partial\boldsymbol{p_t}}{\partial\boldsymbol{q'}}\right)\right)} \quad (217)$$

Here, $\boldsymbol{q_t}$ and $\boldsymbol{p_t}$ are the coordinates and momenta at time $t$ of a classical trajectory started with initial conditions $\boldsymbol{q'}$ and $\boldsymbol{p'}$ at time zero. The integration goes over all initial values $(\boldsymbol{q'},\boldsymbol{p'})$. $S_{\boldsymbol{p'q'}t}$ is the classical action

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