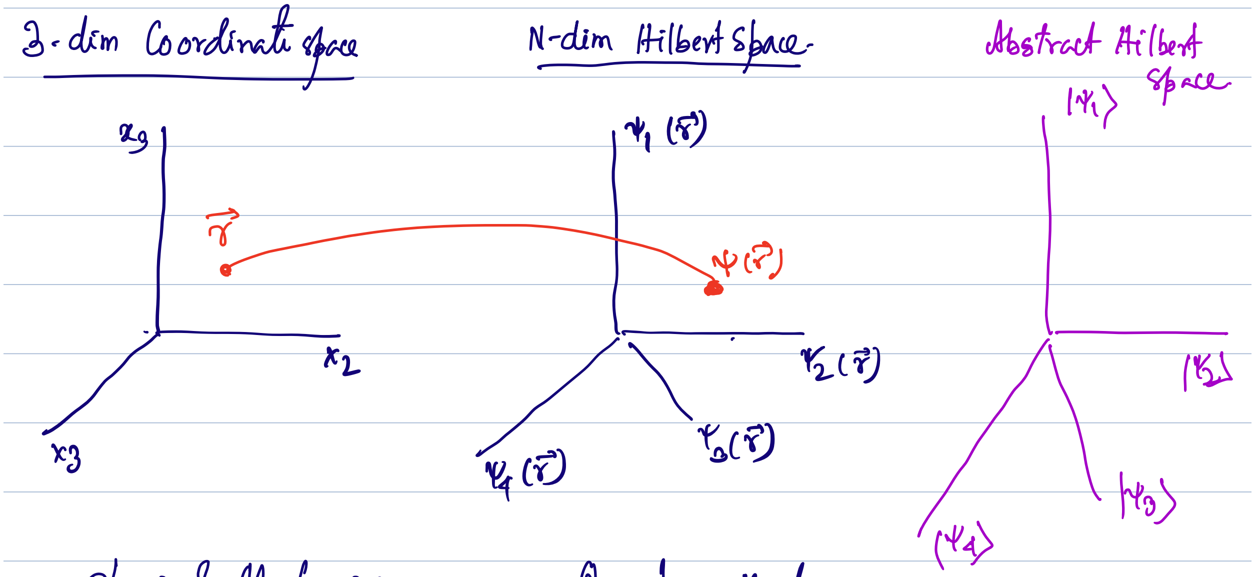
Matrix / Abstract Quantum Mechanics

Let us start with an intuitive and somewhat naive comparative study.



Classical Mechanics.

- In classical mechanics, we define a particle's trajectory by space-time coordinates $\vec{r}(t)$ which can be expressed by three linearly independent unit vectors as

$$\vec{r}(t) = x(t)\,\hat{x} + y(t)\,\hat{y} + z(t)\,\hat{z}.$$

Quantum Mechanics

- In Quantum mechanics, we have a function $\psi(\vec{r},t)$, called wavefunction, which is defined in the space-time domain $(\vec{r},t)$ and is analytic and single valued. The function can also be defined in a basis set of linearly independent functions $\psi_n(\vec{r},t)$ - called Hilbert space. The most convenient basis set is the energy eigenfunctions: $H\psi_n(\vec{r},t) = E_n\psi_n(\vec{r},t)$.

and $\psi(\vec{r},t) = \sum_n c_n(t)\,\psi_n(\vec{r},t)$

We are essentially now going to define an abstract Hilbert / vector space without specifying any domain. We will denote such a set of linearly independent abstract eigenstates/eigenvectors by $|\psi_n\rangle$, also called the ket vectors as $\hat{H}|\psi_n\rangle = E_n|\psi_n\rangle$, and a general ket state is then defined as $|\psi\rangle = \sum_n c_n|\psi_n\rangle$ where c_n are complex numbers. These ket states have no physical meaning as such but the advantage is that you can choose your domain whatever you like such as space-time, or momentum-frequency etc. The procedure to do that (briefly) is to define the ket states in the domain. For example, in the position domain we have position kets which are the eigenvectors of the position operator as $\hat{x}|x\rangle = x|x\rangle$, where x is a number denoting a position in the coordinate space and then we obtain the wave function $\psi(x)$ in the schrödinger equation as $\langle x|\psi\rangle = \psi(x)$. We need to define what is $\langle x|$ state.

- For every position, there is a conjugate space, called the momentum space. We essentially define the trajectory in the position-momentum space – the phase space.

- We don't really measure a vector, but we measure its magnitude and direction. The magnitude is defined as

$$|\vec{r}| = \vec{r}\cdot\vec{r}$$
$$= x_1^2\,\hat{x}_1\cdot\hat{x}_1 + \cdots$$

(where $x_{1,2,3} = x, y, z$)

- The analogy we have in a function is the complex conjugation $\psi_n^*(x)$.

A Hilbert space is defined with all "ket" vectors $|\psi_n\rangle$ which have "conjugate" states – called the dual space and denoted by a "bra" vector $\langle\psi_n|$. Then the general state $\langle\psi|$ is defined as

$$\langle\psi| = \sum_n c_n^* \langle\psi_n|$$ where c_n^* is the complex conjugate of c_n. So, in most cases, the dual space is defined by the Hermitian conjugate '$\dagger$' (transpose + complex conjugation for matrix, vector).

- For a complex function, we also define its amplitude and phase. The amplitude is defined by $S(\vec{r}) = \psi^*(\vec{r})\,\psi(\vec{r}) = |\psi(\vec{r})|^2$.

Then we had the orthonormal condition

$$\int_{-\infty}^{\infty} d\vec{r}\;\psi_n^*(\vec{r})\,\psi_m(\vec{r}) = \delta_{mn}$$ for the basis or eigenstates.

The unit vectors are orthogonal as defined by $\hat{x}_2 \cdot \hat{x}_j = \delta_{ij}$

- In the domain-free abstract Hilbert space, we have the amplitude defined by the inner/scalar product $\langle \psi_n | \psi_m \rangle = \delta_{nm}$, for orthonormal eigenstates. The general state's amplitude is denoted by

$$\langle \psi | \psi \rangle = |\psi|^2 = \sum_{m,n} c_m^* c_n \langle \psi_m | \psi_n \rangle$$

$$= \sum_n |c_n|^2$$

How do we retrive the wavefunction $\psi(x)$?.

We have an Hilbert space for the Hamiltonian $\hat{H}|\psi_n\rangle = E_n |\psi_n\rangle$. Then we want to know the wave function in the position domain which also has an abstract Hilbert space, made of the eigenstates of the position operator $\hat{x}|x\rangle = x|x\rangle$, where x is the position of the particle. Then we write.

$$|\psi_n\rangle = \int dx \, \langle x | \psi_n \rangle \, |x\rangle$$

$$= \int dx \, \psi_n(x) \, |x\rangle$$

where we have the energy eigenvector Hilbert space is discrete (finite or infinite);

and the position eigenvector $|x\rangle$ as continuous and infinite dimensional.

On the otherhand, if we have our domain in the momentum space, we have the corresponding Hilbert space defined by the eigenvectors of the momentum operator as $\hat{p}|p\rangle = p|p\rangle$, with p being its eigenvalue. Then the wavefunction in the momentum space is defined similarly as

$$|\psi_n\rangle = \int dp \, \langle p|\psi_n\rangle \, |p\rangle$$
$$= \int dp \, \psi_n(p) \, |p\rangle .$$

Note that $\psi_n(x)$ & $\psi_n(p)$ are related to each other by the Fourier transformation. This is because the position & momentum space are related to each other being conjugate variables and have uncertainty relation between them. This corresponds to the fact that $\langle \vec{r}|\vec{p}\rangle = e^{i\vec{p}\cdot\vec{r}}$. We will see that more later.

[A cautionary statement about the analogy of the dual state $\langle\psi_n|$ with the momentum conjugate state in the domain. We actually should not be making this analogy to either of them and consider the dual space as it is. In quantum mechanics I & II courses, the dual space is just a Hermition conjugate ($\psi^\dagger$) of the "ket" state. In quantum field theory course, in certain cases, we will find the dual space has the interpretation of a "conjugate momentum" to ψ fields.]

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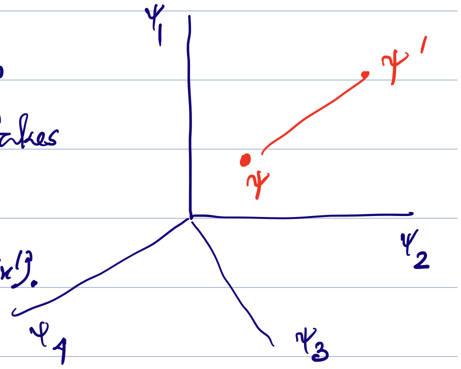
- An operator is something that takes a function $\psi(x)$ to another function $\psi'(x')$. If x, x' are same, then it's a local operator, otherwise it's a non-local operator. e.g. the differentiation is a non-local operator which relates the two functions ψ, ψ' separated in the domain by infinitesimal translation $x' = x + \delta x$ with $\delta x \to 0$. In quantum mechanics, Hermitian operators have an important role. All



observables correspond to the expectation value of the operator in the Hilbert space. If the operator commutes with the Hamiltonian, then they share the same eigenfunctions and the corresponding eigenvalues of the operator are its observable.

- The operator O in the abstract Hilbert space has the same role. It acts on the ket state $|\psi\rangle$ and gives another ket state $|\psi'\rangle$. In the (discrete or continuous) Hilbert space, the operator is a square matrix of $N \times N$ dimension where N is the dimension of the Hilbert space made of N-ket vectors, each ket vector also has N components. The expectation value is defined similarly as $\langle\psi|\hat{O}|\psi\rangle$. This can be denoted in any domain as

$$\int dx\,dx' \underset{\downarrow}{\langle\psi|x\rangle} \underbrace{\langle x|O|x'\rangle}_{\downarrow} \underbrace{\langle x'|\psi\rangle}_{\downarrow}$$

$$= \int dx\, \psi^*(x)\; O(x)\; \psi(x).$$

where we have inserted a complete set $\mathbb{I} = \int dx\, |x\rangle\langle x|$ and we assumed O is a local operator here. You can do it in any other domain. (In the above definition, it's easy to retrieve the interpretation of the expection value as "statistical" average value with $\rho(x) = \psi^*(x)\,\psi(x)$ being the probability density.)

Linear Vector space

What we have seen so far is that a quantum system is described by a Hamiltonian operator $\hat{H}$, with a corresponding wavefunction $\psi(x)$ and energy E. One of the postulates of quantum mechanics is that the wavefunction contains all information about the system. We can associate a probability density $\rho(x) = \psi^*(x)\,\psi(x)$ with the wavefunction's amplitude and the total probability of finding the particle in the entire space is 1. This means $\int_{-\infty}^{\infty} \rho(x)\,dx = \int_{-\infty}^{\infty} \psi^*\psi\,dx = 1$. This says the wave function must be <u>square integrable</u>. Then for every observable we have a linear operator whose expectation value is the measurment result and defined by $\langle O \rangle = \int_{-\infty}^{\infty} dx\; \psi^*(x)\, \hat{O}(x)\, \psi(x)$. A particle of arbitrary energy E in a given system H is associated with a wavefunction $\psi(x)$ such that $E = \int_{-\infty}^{\infty} \psi^*(x)\, \hat{H}\, \psi(x)\, dx$. How do we solve for a general wavefunction $\psi(x)$?

According to linear vector space, any square integrable function can be expanded in a set of orthogononal (linearly independent), normalized (unit amplitude) basis functions (state - called the vector space. (This is analogous to the expansion of a vector in a coordinate system of orthogonal, unit vectors). If the basis functions are eigenfunction of any Hermitian operator, then these basis functions are linearly independent, normalizable, complete set of function, the corresponding vector space is called the Hilbert space. So, we can expand the general wave function $\Psi(x)$ in any Hilbert space that is convenient to us. So, whats the most convenient Hilbert space of a system?

The Hamiltonian $\hat{H}$ is a Hermitian operator and therefore it has a complete set of eigenstates $\Psi_n(x)$ with energy eigenvalues E_n which form a Hilbert space:

$$H\Psi_n(x) = E_n \Psi_n(x) \quad ---(1)$$

, where n are usually discrete set of integers as $n = 0, 1, \cdots N$ (can in principle be negative). N is called the dimension of the Hilbert space which can be finite or infinite. So we can expand $\Psi(x)$ in the energy Hilbert space

$$\Psi(x,t) = \sum_n c_n(t)\, \Psi_n(x,t). \quad ---(2)$$

where the expansion coefficients c_n are complex, in general, and is given by

$$c_n = \int_{-\infty}^{\infty} dx \;\; \Psi_n^*(x)\, \Psi(x) \quad ---(3)$$

c_n is the probability amplitude of the general state $\Psi(x)$ to be in the n^{th} state. Since Ψ is normalized to one and $\Psi_n(x)$ are orthonormal, i.e. $\int_{-\infty}^{\infty} \Psi_n^*(x)\, \Psi_m(x)\, dx = \delta_{nm}$, so, $\sum_n |c_n|^2 = 1$, i.e, the total probability of finding the particle in all the eigenstates in the entire space is 1.

Therefore, solving a Schrödinger equation means solving the energy eigenvalue eq (1). But unfortunately, solving eq(1) is not always easy, especially for complicated potential $V(x)$ and when many particles are present. Therefore, although energy Hilbert space is indeed the most convenient Hilbert space, but its not always available to us. What other Hilbert space can be helpful?

We have already used another Hilbert space, i.e., the Hilbert space of a momentum operator $\hat{p}$. This Hilbert space is also the eigenstates of the kinetic energy operator of the Hamiltonian $\hat{H} = \hat{K} + \hat{V}$, became $\hat{K} = \frac{\hat{p}^2}{2m}$. This Hilbert space is called the plane wave basis state, because its the eigenstates of the free particle. (Its not a Hilbert space in the strick sense because plane waves are not normalizable, and we need some boundary condition, e.g., box normalization, periodic boundary condition to normalize it). These boundary conditions also restrict the allowed values of momentum or wave vector to discrete values. This made the plane wave Hilbert space discrete and finite or denumerably infinite. Next we constructed a wavepacket, which is a general wavefunction expandend in the plane wave basis as eq(2), with $\psi_{n=k}(x,t) \equiv e^{i(kx-\omega t)}$ and $c_{n=k} \equiv \phi_k$. The coefficients ϕ_n has the same meaning as c_n that it gives the probability amplitude of occupying a given momentum state. Without any potential (free particle) $\phi_k = \delta(k-k_0)$ where k_0 is the only eigenvalue of the momentum operator taken by the particle. On the other hand, $\phi_k = 1$ for all k-values for a delta function potential, in which all possible momentum values are allowed. So, clearly ϕ_k depends on the potential energy and the boundary conditions. As a potential energy is involved with a condition that the energy of the particle is higher and lower in separate parts of space. Then where $E > V$, we have plane wave / oscillatory solutions and where $E < V$, we have negative kinetic energy (imaginary momentum) where the wavefunction decays exponentially. This confines the system and we have discrete energy eigenvalues and wave packet eigenfunctions. One lesson we learned is that we can split our Hamiltonian into two parts $H = H_0 + H'$. Lets say now H_0 can be solved exactly (e.g., the K.E. part) and obtain a Hilbert space; and then the wavefunction of the total Hamiltonian can be expanded in this Hilbert space. In this choice of Hilbert space, atleast some part of the Hamiltonian (H_0) is already solved, and for the other part H', we can compute the expectation value to obtain the allowed energies of the theory. This method is called the Perturbation theory that we will learn later.

[When we have a degeneracy in the Hilbert space, say, the nth state has M-fold degeneracy, i.e., same eigenvalue. We express those degenerate states as $(\psi_{n,1}, \psi_{n,2}, \cdots, \psi_{n,M})$, such that $H\psi_{n,m} = E_n \psi_{n,m}$. Then the general nth eigenstate can be written as a linear superposition of those degenerate states as

$$\psi_n(x) = \sum_{m=1}^{M} d_{n,m}\, \psi_{n,m}(x) .$$

This gives

$$\begin{aligned}
H\psi_n &= H \sum_{m=1}^{M} d_{n,m}\, \psi_{n,m}(x) \\
&= \sum_{m=1}^{M} d_{nm}\, H \psi_{n,m}(x) \qquad \text{[since } H \text{ is a linear operator]} \\
&= \sum_{m=1}^{N} d_{nm}\, E_n \psi_{n,m}(x) \\
&= E_n \sum_{m=1}^{N} d_{n,m}\, \psi_{n,m}(x) \\
&= E_n \psi_n .
\end{aligned}$$

This result is a manifestation of the superposition principle, owing to the linear Schrödinger equation, that where there is a degeneracy, the particle has finite probability to occupy all degenerate states, and $|d_{n,m}|$ gives the probability amplitude.]

So, our take home message is that wavefunction $\psi(x)$ encapsulate all information of a particle in a quantum system (H) with a given energy, and we need to find a suitable Hilbert space to expand the wave function.

Dirac Bracket Notation - Abstract Hilbert space

Dirac realized that in choosing the suitable Hilbert space for a wavefunction, the position domain $\vec{r}$ has very little or no role in it. So far in all examples in the previous chapter, the position domain actually played important role since it contains the potential profile and dictated the normalization condition. Then normalization condition was important for obtaining quantized energy eigenvalues and eigenfunction.

- Dirac relaxed the normalizability condition in the entire space to general normalization condition or inner product or scalar product notation as

$$\langle \psi_1 | \psi_2 \rangle \equiv \int_{-\infty}^{\infty} dx \; \psi_1^*(x) \, \psi_2(x) \qquad -(1)$$

for any two abstract quantities $|\psi_2\rangle$ and $\langle \psi_1|$ which are like column and row vectors, respectively. They are called 'ket' and 'bra' vectors and they are abstract / formal mathematical objects. Their physical interpretation, in terms of measurable or not, is perhaps not present, apart from column & row vectors of N-dimension. However, they take the shape of wavefunctions $\psi_2(x) = \langle x | \psi_2 \rangle$ and $\psi_1^* = \langle \psi_1 | x \rangle$ where $|x\rangle$ is the ket vector of the position operator (to be clarified later). If $|\psi_1\rangle$ is the ket vector and

$\langle\psi|$ is its corresponding "bra" vector, called the dual space by which the inner product (normalization) is defined. Mathematicians have figured out the abstract algebra of these quantities, each algebra can be reproduced if we treat ket & bra states as column and row vectors or if we take a projection to any domain (like position), we reproduce all algebra by the wavefunctions.

- $\langle\psi_1|\psi_2\rangle = \langle\psi_2|\psi_1\rangle^*$
- $\langle\psi_1|c\psi_2\rangle = c\langle\psi_1|\psi_2\rangle$ for any complex number c.
- $\langle c\psi_1|\psi_2\rangle = c^*\langle\psi_1|\psi_2\rangle$
- $\langle\psi_3|\psi_1+\psi_2\rangle = \langle\psi_3|\psi_1\rangle + \langle\psi_3|\psi_2\rangle$
- $|\psi_1\rangle$ and $|\psi_2\rangle$ are said to be orthogonal if their inner product vanishes, ie, $\langle\psi_1|\psi_2\rangle = 0$
- $|\psi_1\rangle$ is said to be normalized if $\langle\psi_1|\psi_1\rangle = 1$.
- We can combine the last two conditions into the orthonormal condition for a set of ket states/vectors $|\psi_n\rangle$ as

$$\langle\psi_n|\psi_m\rangle = \delta_{mn}.$$

- Operators.

Heisenberg and Dirac realized that square Hermitian matrices also have eigenvalues and eigenfunctions. Therefore, Hamiltonian can also be represented as matrix, which takes a vector and gives another vector from the matrix algebra.

An operator is an abstract object which acts on a ket state/vector and gives another ket vector (As we project the ket states and operators into a specific domain, then the operators have the physical meaning of acting on a wavefunction and gives another wavefunction, like differential operator, momentum operator, Hamiltonian etc. Similarly the expectation value has to be generalized to inner product as seen below).

- So, another postulate of quantum mechanics is that every dynamical variable is associated with a linear operator in the abstract space (An observable / measurable quantity is a special dynamical variable which is associated with a Hermitian operator).

So, an operator gives $\hat{A}|\psi_1\rangle = |\psi_2\rangle$. Sometimes, $|\psi_2\rangle$ is written as $|\psi_2\rangle = |A\psi_1\rangle$, i.e., $\hat{A}|\psi_1\rangle = |A\psi_1\rangle$. An operator is said to be linear if it satisfies the following property

$$\hat{O}\left(c_1|\psi_1\rangle + c_2|\psi_2\rangle\right) = c_1\,\hat{O}|\psi_1\rangle + c_2\,\hat{O}|\psi_2\rangle$$

for any two complex numbers c_1 & c_2 and any states $|\psi_1\rangle, |\psi_2\rangle$.

The expectation value of this operator between any two states $|\psi_1\rangle$ and $|\psi_2\rangle$ is

$$\langle \psi_1 | \hat{A} | \psi_2\rangle = \langle \psi_1 | \hat{A}\psi_2\rangle = \langle \hat{A}^{+}\psi_1 | \psi_2\rangle$$

$$\left(\text{in the } x\text{-domain} \quad \equiv \int_{-\infty}^{\infty} dx \; \psi_1^{+}(x)\, \hat{A}\, \psi_2(x) = \int_{-\infty}^{\infty} dx \, (A^{+}\psi_1)^{+} \psi_2 \right)$$

where we have used the identity $\langle \psi_1 | A\psi_2\rangle = \langle \hat{A}^{+}\psi_1 | \psi_2\rangle$.

Lets try to calculate

$$\langle \psi_1 | A | \psi_2\rangle^{+} = \left(\int dx \; \psi_1^{+} A \psi_2 \right)^{+}$$

$$= \int dx \; \psi_2^{+} A^{+} \psi_1 = \langle \psi_2 | A^{+} \psi_1\rangle$$

$$= \langle A\psi_2 | \psi_1\rangle.$$

(whenever $+$ acts on a function and scalar number, it simply gives the complex conjugation $*$).

- Eigenvalue and Eigenvector: A ket vector $|\psi_n\rangle$ is said to be an eigenket or eigenvector of an operator $\hat{A}$ if $\hat{A}$ acting on $|\psi_n\rangle$ produces the same ket vector $|\psi_n\rangle$ as

$$\hat{A} |\psi_n\rangle = a_n |\psi_n\rangle \quad \cdots (5)$$

where a_n is the corresponding eigen (proper) value which is in general a complex number. Taking Hermitian conjugate on both sides we get

$$\langle \psi_n | \hat{A}^{+} = a_n^{*} \langle \psi_n | \quad -- (6)$$

We see that if $|\psi_n\rangle$ is an eigenvector of $\hat{A}$ with eigenvalue 'a_n', then $\langle \psi_n|$ is the dual eigenvectors of A^{+} with the eigenvalue

a_n^*. In the above expression $|\psi_n\rangle$ & $\langle\psi_n|$ are also called right and left eigenvectors.

- a_n is said to be one of the proper / precise result of a measurement of the dynamical variable / operator $\hat{A}$. Because its an eigenvalue, this value has no uncertainty or variance. It can be checked easily. The uncertainty / variance is defined as $\langle \Delta A \rangle = \langle \psi_n | \Delta A | \psi_n \rangle = \sqrt{\langle A^2 \rangle - \langle A \rangle^2}$, where $\langle A \rangle = \langle \psi_n | A | \psi_n \rangle = a_n$ and $\langle A^2 \rangle = \langle \psi_n | A^2 | \psi_n \rangle = a_n^2$. So, $\langle \Delta A \rangle = 0$.

- The totality of the eigenvalues of an operator is called the spectrum of that operator. One can have discrete n or continuous n values and also the total number of eigenvalues can be finite or infinite. In all the examples we have seen in the previous chapter, the spectrum of the Hamiltonian, ie, the eigenvalues are discrete and infinite.

- **Hermitian Operators :** Since the results of measurements are real numbers, so we will only concern ourselves with those operators which are guaranteed to give real eigenvalues. We can figure out the constraint on the operators which guarantee to give real eigenvalues from eqs (5) and (6) : Since $a_n^* = a_n$, we have

$$\boxed{A^+ = A} \qquad -- (7)$$

These operators are called self-adjoint or Hermitian operators. Its called self-adjoint because the operator '+' is also called adjoint operation or Hermitian conjugation.

Not only the eigenvalues, but the expectation values of the Hermitian operator on any general state is also real. Lets consider $\langle A\rangle^+ = \langle\psi|A|\psi\rangle^+ = \langle\psi|A^+|\psi\rangle = \langle\psi|A|\psi\rangle = \langle A\rangle$.

All physical operators in Quantum Mechanics are Hermitian operators. Lets check for the momentum operator in the position space $\hat{p} = -i\hbar\frac{\partial}{\partial x}$. $\hat{p}^+ = i\hbar\left(\frac{\partial}{\partial x}\right)^*$, so it does not look Hermitian. But you have to see how derivative operator acts on the state. Lets see an example :

$$\frac{\partial\psi}{\partial x} = \lim_{\varepsilon\to 0}\frac{\psi(x+\varepsilon)-\psi(x)}{\varepsilon}.$$

$$\left(\frac{\partial\psi}{\partial x}\right)^* = \lim_{\varepsilon\to 0}\frac{\psi^*(x+\varepsilon)-\psi^*(x)}{\varepsilon}. = \frac{\partial}{\partial x}\psi^*$$

So, when a derivative operator acts on a wave function ψ, its Hermitian conjugation acts on ψ^*. That what $\left(\frac{\partial}{\partial x}\right)^*$ notation stands for.

Once we incorporate that, we can prove that $\langle \psi | \hat{p} | \phi \rangle = \langle \psi | \hat{p}^{+} | \phi \rangle$ when $\hat{p}$ acts on ϕ and $\hat{p}^{+}$ acts on ψ.

How about the energy operator $\hat{E} = i\hbar \frac{\partial}{\partial t}$ and $\hat{E}^{*} = -i\hbar \left(\frac{\partial}{\partial t}\right)^{*}$

For most other operators we do not have to worry about it much. Only for those operators having 'i' is little subtle.

- **Product of operators:** Let A, B two linear operators, their product is defined by $(AB)|\psi\rangle = A(B|\psi\rangle)$, in which B acts first on ψ and then A acts on the new state $(B|\psi\rangle)$. In general $AB \neq BA$. The difference between their product is called the commutator and is defined by

$$[A,B] = -[B,A] = AB - BA.$$

- $(AB)^{+} = B^{+}A^{+}$; $(cA)^{+} = A^{+}c^{*} = c^{*}A^{+}$ where c is complex number.
- **Functions of operators:** Much like how the function of a variable can be expanded in power series (analytic function), we can expand the function of an operator as

$$f(\hat{A}) = \sum_{i=0}^{\infty} c_i \hat{A}_i$$

, where c_i are complex numbers.

Then if ψ_n satisfies $\hat{A}|\psi_n\rangle = a_n|\psi_n\rangle$, then $f(A)|\psi_n\rangle = f(a_n)|\psi_n\rangle$.

The adjoint of $f(A)$ is $[f(A)]^{+} = \sum_{i=1}^{\infty} (c_i A_i)^{+} = \sum_{i=1}^{\infty} A_i^{+} c_i^{*} = f^{*}(A^{+})$.

Popular functions of operator that we use are e^{A}, $\sin A$, $\cos A$, etc.

Then $e^{A}e^{B} = e^{A+B+\frac{1}{2}[A,B] + \frac{1}{12}[A,[A,B]] - \cdots}$

This is called Baker-Cambell-Hausdorff formula.

- **Projection operators:** A Hermitian operator P is said to be a projection operator if $\boxed{P^2 = P}$. If we apply P on a state $|\psi_n\rangle$ it gives a new state $|\psi_n'\rangle = P|\psi_n\rangle$. Then apply again $P|\psi_n'\rangle = P^2|\psi_n\rangle = P|\psi_n\rangle$. A much used projection operator is $P = |\psi_n\rangle\langle\psi_n|$.

Any state $|\psi\rangle$ can be written in terms of two linearly independent (orthogonal) states $|\phi\rangle$ + $|\chi\rangle$, where $\langle\phi|\chi\rangle = 0$, by means of a projection operator P as $|\phi\rangle = P|\psi\rangle$ or $P = |\phi\rangle\langle\psi|$ and $|\chi\rangle = (\mathbb{I} - P)|\psi\rangle$. Then we have

$$|\psi\rangle = |\phi\rangle + |\chi\rangle.$$

Now, $\langle\phi|\chi\rangle = \langle P\psi|(\mathbb{I}-P)\psi\rangle = \langle\psi|(P-P^2)|\psi\rangle = \langle\psi|(P-P)|\psi\rangle = 0$

since P is Hermitian and $P^2 = P$. Note that $\mathbb{I} - P$ is also a projection operator.

- **Ladder operator** (Also called Raising / Lowering operator).

The operator

$$L = |\psi_n\rangle\langle\psi_m| \quad \text{for } n \neq m \text{ and}$$

$|\psi_n\rangle$ and $|\psi_m\rangle$ belong to the same Hilbert space, is called the Ladder operator. It acts on the $|\psi_m\rangle$ state and takes us to the $|\psi_n\rangle$ state. Clearly, $L^2 = 0$.

• Inverse and Unitary operators:

The unit operator I is the operator that leaves any function ψ unchanged : $I\psi = \psi$.

If A, B are two linear operators which satisfy $AB = BA = I$, then $B = A^{-1}$ is said to be the inverse operator of A.

An operator is said to be unitary if it satisfies

$$U^{-1} = U^{\dagger} \Rightarrow UU^{\dagger} = U^{\dagger}U = I.$$

→ A unitary operator can be expressed in the form $U = e^{iA}$, where A is a Hermitian operator: $U^{\dagger} = (e^{iA})^{\dagger} = e^{-iA^{\dagger}} = e^{-iA}$.

→ Multiplication of a ket vector by a unitary operator leaves the inner product and expectation values unchanged. Let's say $|\psi\rangle$ is a state which is transformed by a unitary transformation U to $|\psi'\rangle = U|\psi\rangle$. Then $\langle\psi| \to \langle\psi|U^{\dagger}$. So we get

$$\langle\psi'|\psi'\rangle = \langle\psi|\underbrace{U^{\dagger}U}_{I}|\psi\rangle = \langle\psi|\psi\rangle.$$

$$\langle\psi'|A'|\psi\rangle = \langle\psi|U^{\dagger}A'U|\psi\rangle = \langle\psi|A|\psi\rangle$$

where an operator transforms under the unitary transformation as $A' = UAU^{\dagger}$. (H.W. Show that if A is hermitian, so does A').

→ Operator equations remain unchanged under a unitary transformation. Let us consider an operator equation

$$f(A,B,C) = c_1 A + c_2 BC .$$

$A \to A' = UAU^\dagger$, and so on, c_1, c_2 are complex numbers. Then

$$f(A',B',C') = U\, f(A,B,C)\, U^\dagger = c_1 \underbrace{U A U^\dagger}_{A'} + c_2\, U B \underset{\text{insert } U^\dagger U = I}{\uparrow} C\, U^\dagger$$

$$= c_1 A' + c_2 B'C'.$$

So, commutator relations remain unchanged: $[A,B] = [A',B']$.
Eigenvalue equations, equation of motion remain unchanged.
e.g. The time-independent Schrödinger equation:

$$H|\psi_n\rangle = E_n|\psi_n\rangle \to H'|\psi_n'\rangle = E_n|\psi_n'\rangle.$$

where $H' = UHU^\dagger$ & $|\psi_n'\rangle = U|\psi_n\rangle$, where U is <u>any</u> unitary transformation. Eigenvalues E_n remains the same. So does the expection values as shown earlier. This is also simply because any scalar numbers remain unchanged under a unitary transformation: $UcU^\dagger = cUU^\dagger = c$. Only vector changes as $|\psi\rangle \to U|\psi\rangle$ and operator chanes as $A \to UAU^\dagger$.
For the same reason, a wavefunction $\psi(x)$ remain unchanged since its a complex number and expressed as an inner product $\psi(x) = \langle x|\psi\rangle$ where $|x\rangle$ is the position eigenvector (see below)

The time-dependent Schrödinger equation also remains unchanged: $-i\hbar \frac{\partial}{\partial t}|\psi\rangle = H|\psi\rangle \to -i\hbar \frac{\partial}{\partial t}|\psi'\rangle = H'|\psi'\rangle$.

⊛ If we define $U(t,t_0)$ as a unitary operator, it leaves the inner product, i.e., probability density constant in time at all time. This is one of the fundamental postulates of quantum mechanics:

$$\langle \psi(t)|\psi(t)\rangle = \langle \psi(t_0)|\underbrace{U^{\dagger}(t,t_0)\, U(t,t_0)}_{I}|\psi(t_0)\rangle$$

$$= \langle \psi(t_0)|\psi(t_0)\rangle$$

$$= \text{A constant in time.}$$

Ex 1. The gauge transformation or phase arbitrariness of the wave fn. that we defined before and said to leave the quantum system invariant is an example of unitary transformation $\psi \to \psi' = e^{i\theta}\psi$.

Ex2: The solution of time-dependent schrödinger equation $i\hbar \frac{\partial}{\partial t}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle$ gives.

$$|\psi(t)\rangle = e^{i\frac{\hat{H}(t-t_0)}{\hbar}}|\psi(t_0)\rangle = \hat{U}(t,t_0)|\psi(t_0)\rangle \quad --(8)$$

where we have assumed time independent Hamiltonian. Therefore, $\hat{U}(t,t_0) = e^{i\hat{H}(t-t_0)/\hbar}$ is a unitary operator (a fn. of $\hat{H}$) which takes a ket vector at t_0 to another ket vector at t. Therefore, the unitary transformation defined in this way gives a time translation or time evolution of the state vector. This is consistent with what we learned in classical mechanics that if time-translation is a symmetry, then the Hamiltonian (energy) is conserved (Noether's theorem). Therefore, any conserved quantity generates a translation of the corresponding conjugate variable. And the translation or evolution of that variable is generated by a unitary operator.

Ex3: Following the above example, its easy to generalize the above form of unitary operator for time translation / evolution to other unitary operators which generate space translation, angular translation (rotation) and so on. Its clear that the unitary operator made of domain variable and its conjugate operator can be the right choice.

Lets take the ansatz $U(x,x_0) = e^{i\hat{p}(x-x_0)/\hbar}$ as a unitary operator for spatial translation. Note that in the exponential $\hat{p}$ is an operator and $x-x_0$ are scalar variable. We demand that $\psi(x) = U(x,x_0)\,\psi(x_0)$. To prove that we use the position representation of the momentum operator $\hat{p} = -i\hbar\frac{\partial}{\partial x}$. Then we have

$$e^{(x-x_0)\frac{\partial}{\partial x}}\psi(x_0) = \sum_{n=0}^{\infty}\frac{(x-x_0)^n}{n!}\frac{\partial^n}{\partial x^n}\psi(x_0)$$

$$= \psi(x_0) + (x-x_0)\frac{\partial\psi}{\partial x}\Big|_{x=x_0} + \frac{(x-x_0)^2}{2!}\frac{\partial^2\psi}{\partial x^2}\Big|_{x=x_0} + \cdots$$

The R.H.S is the Taylor series of $\psi(x)$ w.r.to x_0.

$$= \psi(x).$$

Therefore, its proven that $U(x,x_0)$ indeed make a displacement of ψ from x_0 to x. (We know that a derivative operator generates an infinitesimal displacement. So $U(x,x_0)$ is actually a product of infinite number of infinitesimal displacements between x to x_0. This is the manifestation of a continuous symmetry.

[H.W. . Show that $U(\theta,\theta_0) = e^{i\hat{L}(\theta-\theta_0)/\hbar}$ makes a rotation of a state $\psi(\theta_0)$ to $\psi(\theta)$. $\hat{L}$ is the angular momentum along the axis of rotation. We also see a common property that that the form of the canonical conjugate operator for a general variable q is defined in quantum mechanics by $i\hbar\frac{\partial}{\partial q}$, where $q = t, x, \theta$ etc whose conjugate operators $\hat{H}, \hat{p}, \hat{L}$.]

• Eigenstates and Hilbert space.

We now revisit the eigenvalue & eigenstates problem for linear, Hermitian operators which make up the dynamical variables of quantum mechanics. Let $\hat{A}$ be a linear, Hermitian operator (such as the Hamiltonian $\hat{H}$, momentum $\hat{p}$, position $\hat{x}$, etc) which have a set of real eigenvalues 'a_n' and corresponding abstract eigenvectors $|\psi_n\rangle$

$$\hat{A}\,|\psi_n\rangle = a_n\,|\psi_n\rangle \qquad \cdots (9)$$

The index 'n' can be discrete or continuous, and can have a finite or infinite total number of eigenstates.

For the linear, Hermitian operator $\hat{A}$, its eigenvalues and eigenfunctions obey the following properties:

(a) All eigenvalues 'a_n' are real.

(b) The eigenvectors $|\psi_n\rangle$ are normalizable, which is also called square integrable.

$$\langle\psi_n|\psi_n\rangle = 1. \qquad ----(10)$$

(If we solve the eigenvalue equation, we may not immediately obtain '1' on the R.H.S. but we may get some complex numbers, say c_n. But then we can divide the ket and bra states by $|\psi_n\rangle \to \frac{1}{\sqrt{c_n}}|\psi_n\rangle$, and $\langle\psi_n| \to \frac{1}{\sqrt{c_n^*}}\langle\psi_n|$. Now since $\hat{A}$ is a linear operator, any constant multiplications to eq (9) does not change the eigenvalue equation. So, without loosing generality we can write eq (10).)

(c) Orthogolality: One of the important property of the eigenvectors of a Hermitian, linear operator is that all the eigenvectors are linearly independent (i.e. orthogonalizable by the Gram-Schmidt method and hence we simply call them orthogonal). To prove that, we consider any two eigenvectors $|\psi_n\rangle$ and $|\psi_m\rangle$ of $\hat{A}$ with corresponding eigenvalues a_n & a_m, respectively. $\hat{A}\,|\psi_n\rangle = a_n\,|\psi_n\rangle$ & $\hat{A}\,|\psi_m\rangle = a_m\,|\psi_m\rangle$.
Take Hermitian conjugation of the 2nd equation: $\langle\psi_m|\,A^\dagger = a_m^* \langle\psi_m|$ and subtract the first equation

$$\langle\psi_m|\,(\hat{A}^\dagger - \hat{A})\,|\psi_n\rangle = \langle\psi_m|\,(a_m^* - a_n)\,|\psi_n\rangle$$

$$\Rightarrow \quad \langle\psi_m|\,(\underset{\uparrow}{\hat{A}} - \hat{A})\,|\psi_n\rangle = \underset{\uparrow}{(}a_m - a_n)\,\langle\psi_m|\psi_n\rangle.$$

since A is Hermitian since a_m are real numbers.

$$\Rightarrow \quad (a_m - a_n)\,\langle\psi_m|\psi_n\rangle = 0$$

(i) When $a_n \neq a_m$, i.e. the two eigenvalues are not degenerate, we get $\langle\psi_m|\psi_n\rangle = 0$. ---- (11)

Since $|\psi_n\rangle$ & $|\psi_m\rangle$ are any two non-degenerate eigenstates of $\hat{A}$, so, all non-degenerate eigenstates are linearly independent and orthogonal.

(ii) When $a_m = a_n$, i.e. for any two degenerate eigenstates, we can not say anything about whether the two states are orthogonal or not. But any linear combination of of the two degenerate eigenstates $|\Psi\rangle = c_1 |\Psi_n\rangle + c_2 |\Psi_m\rangle$ is also an eigenstate of the linear operator $\hat{A}$. (H.W. Prove this statement). Therefore, even if they are not orthogonal to begin with, from the infinite possible states $|\Psi\rangle$ made of two states we can always construct two linearly independent states which then can be made orthogonal by the Gram-Schmidt method. In other words, we can always choose two linearly independent eigenvectors for the two-fold degenerate states.

This statement is general for any m-fold degenerate case in which any linear combination of the m-degenerate states is an eigenstate and hence we can construct m-linearly-independent eigenstates.

The total number of linearly independent eigenstates in a finite(N)dimensional operator (think of an operator as a $N \times N$ matrix here for understanding) is fixed to be N and hence if there is m-fold degeneracy, then there are $N-m$ distinct eigenvalues.

Typically (b) & (c) are combined into the orthonormal condition $\boxed{\langle \Psi_m | \Psi_n \rangle = \delta_{m,n}}$, --- (12)
which is equivalent to normalization condition for $m=n$.

(d) Closure / completeness Property: All the eigenvectors of a linear, Hermitian operator follows the closure / completeness property defined as

$$\sum_n |\psi_n\rangle\langle\psi_n| = \mathbb{I}, \quad --- (13)$$

where the summation n runs over all eigenvectors (say N) and $\mathbb{I}$ is a $N\times N$ unit matrix. This closure relation can be proven but it is often postulated, such that if the eigenvectors of a linear, Hermition is complete, then any square integrable function can be expanded in this basis state, or if a square integrable function can be fully expanded in a given set of eigenstates, then that eigenstates are complete. (Not all Hermitian operators gaurantee to have a complete eigenstates, but those which do correspond to observables / physical quantum operators, and vice versa).

Eq (12) & (13) essentially say that the eigenvectors of a linear, Hermitian operator form a Hilbert Space. Therefore, any general state vector $|\Psi\rangle$ of the same operator can be expanded in the Hilbert space of its eigenvectors:

$$|\Psi\rangle = \sum_n c_n |\psi_n\rangle \quad --- (14)$$

where c_n are the complex number which can be obtained as $c_n = \langle\psi_n|\Psi\rangle$ (show). The interpretation of these coefficients are already given. Suppose the expectation value of the operator A, ie, $\langle A \rangle$ which matches with any one eigenvalue of the operator, say, n^{th} eigenvalue, then $\langle A \rangle = a_n$ and $C_n = 1$ and $C_{m \neq n} = 0$. Then the operator has a precise value. On the other hand if $\langle A \rangle$ does not match with any of the eigenvalue then its generic wavefunction can be written as eq.(4) which says the state $|\psi\rangle$ has finite probability $\propto |C_n|^2$ to be simultaneously present in all states in this Hilbert space and zero probability to be in any other state that is not part of the Hilbert space. This last statement comes from the normalizability of the state $|\psi\rangle$ as $\langle \psi | \psi \rangle = 1 \Rightarrow \sum_n |C_n|^2 = 1$, so the total probability of finiding the state within this Hilbert space is 1.

- If two linear, Hermitian operators commute, ie, $[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A} = 0$, then they share the same eigenstates (and hence the Hilbert space). Suppose $|\psi_a\rangle$ is an eigenstate of $\hat{A}$: $A|\psi_a\rangle = a|\psi_a\rangle$. Then $\hat{A}\hat{B}|\psi_a\rangle = \hat{B}\hat{A}|\psi_a\rangle = \hat{B}(a|\psi_a\rangle) = a(\hat{B}|\psi_a\rangle)$. So, $\hat{B}|\psi_a\rangle$ is also an eigenstate of $\hat{A}$ with the same eigenvalue. Now, $B|\psi_a\rangle$ and $|\psi_a\rangle$, both being the eigenstate of $\hat{A}$ with the same eigenvalue a, so, these two states can either be orthogonal (degenerate case) $\langle \psi_a | B\psi_a \rangle = 0$, or linearly dependent, ie., $\hat{B}|\psi_a\rangle = b|\psi_a\rangle$. For linear operator, the 2nd option works. This means, $|\psi_a\rangle$ is also an eigenstate of $\hat{B}$ with an eigenvalue b. One can hence attach two quantum numbers $|\psi_{a,b}\rangle$ to each eigenstate in the Hilbert space.

Continuous Spectrum:

When the index 'n' is a continuous variable, as we will see, for example, for position, momentum operators whose eigenvalues are continuous and hence eigenvectors are continuous spectrum, the normalization and closer relations modify to

$$\langle \psi(s) | \psi(s') \rangle = \delta(s-s') \quad \text{---}(12')$$

$$\int ds \, |\psi(s)\rangle\langle\psi(s)| = \mathbb{I}, \quad \text{---}(13')$$

$$\text{so that} \quad \int ds \, \langle\psi(s)|\psi(s)\rangle = 1.$$

where s is the variable of the eigenvectors. Notice that for a continuous variable, it is customary to write it in the bracket in a function, while for discrete variable, we call it index, we write it as subscript or superscript. Eq(13') is also sometimes called resolution operator/relation.

Hilbert Space in QM: Since in quantum mechanics, we deal with wavefunction, which is a complex function defined in the domain of position, momentum, time etc, we need to find the suitable Hilbert space for the wavefunction to be expanded. So fare in the previous chapters, we have solved the eigenvalue equation of the time-independent Schrödinger equation in the position domain. The normalizibility condition and the continuity of wavefunction and its 1st derivative gave us the quantization criterion of discrete set of energy eigenvalues and eigenfunctions. Specific to the 2nd order differential equation of the Schrödinger equations, we always get two sets of linearly independent solutions. But we often end up using one of them, because thats the normalizable solution. Since normalizibility / square integrability is a criterion of the Hilbert space, so all normalizable eigenstates form a Hilbert space.

Let us consider a system defined by a domain-free abstract Hamiltonian operator $\hat{H} = \hat{K} + \hat{V}$, which has a Hilbert space $|\psi_n\rangle$ with energy eigenvalues $\hat{H}|\psi_n\rangle = E_n|\psi_n\rangle$. --- (11)

Then if we now add a particle with a fixed energy E into the system defined by its Hamiltonian $\hat{H}$, then the particle assumes a state vector $|\psi\rangle$ which is defined by the condition $\langle\psi|\hat{H}|\psi\rangle = E$. Then the particles position, momentum etc are determined similarly by $\langle\psi|\hat{x}|\psi\rangle$, $\langle\psi|\hat{p}|\psi\rangle$. Determination of $|\psi\rangle$ becomes easier if we choose the right Hilbert space. If we expand $|\Psi\rangle$ in the eigenenergy Hilbert space we have

$$|\Psi\rangle = \sum_n c_n |\Psi_n\rangle . \quad \cdots (14).$$

We get two conditions. (i) $\langle\Psi|\Psi\rangle = 1 \Rightarrow \sum_n |c_n|^2 = 1$.

(ii) And, we have $H|\Psi\rangle = \sum_n c_n H|\Psi_n\rangle = \sum_n c_n E_n |\Psi_n\rangle = E|\Psi\rangle$, such that $E = \sum_n |c_n|^2 E_n$. Therefore, the particle gets "distributed" among different energy eigenstates under two constraints that the total probability of being the particle in this Hilbert space is 1, and the total energy E is conserved. If the energy of the particle matches with any energy energy eigenvalue, then the wave function $|\Psi\rangle$ will coincide with that eigenstate, say $|\Psi_n\rangle$ and the corresponding coefficient $c_n = 1$ and $c_{m\neq n} = 0$. Otherwise, for any general energy value E, this is an average/expectation value of the Hamiltonian. This means there is a variance/uncertainty in its value $\Delta E = \sqrt{\langle H^2\rangle^2 - \langle H\rangle^2}$, where $\langle H\rangle = \sum_n |c_n|^2 E_n$. $\langle H^2\rangle = \langle\Psi|H^2|\Psi\rangle = \sum_n |c_n|^2 E_n^2$. Clearly $\Delta E \neq 0$. Therefore, the time uncertainty $\Delta t \neq \infty$. This means, the values of c_n are not fixed but c_n is time dependent, but the (i) normalization condition & (ii) total energy condition remain time-independent. (To evaluate their time dependence, we need to invoke time-dependent Schrödinger equation. So simple time independent Schrödinger equation, its easy to solve $c_n(t) = c_n(0)\, e^{-iE_n t/\hbar}$)

A digression to Quantum Statistical Mechanics :

Another possibility we can think of adding a heat bath to the system such that the particles energy changes by k_BT, but the system's Hamiltonian and hence the Hilbert space remain unchanged. Therefore, since the energy of the particle E is changing with temperature and so does the wavefunction $|\psi\rangle$, where H, $|\psi_n\rangle$, E_n are fixed. Therefore, the coefficients c_n become temperature dependent. With different temperature, the particle's wavefunction's distribution or probability amplitude into different eigenstates changes such that the (i) normalization and (ii) average energy conditions remain unchanged. This actually becomes a quantum statistical mechanics problem now where we have to now minimize the free energy with the constraints of (i) & (ii). The Lagrangian multiplier to implement the normalization condition turns out to be $\beta = 1/k_BT$. But there are many possible values or configurations of c_n which satisfy conditions (i) & (ii) - which gives the entropy term. This gives a partition function and Boltzmann distribution function which sums over all possible values of c_n under the constraints (i) & (ii) leading to an entropy term and hence a free energy $F = \langle H\rangle - TS$. The idea is to maximize the entropy to minimize F (thermal equilibrium). After solving the free energy one obtains $|c_n|^2 \sim e^{-\beta E_n}$ (called Maxwell Boltzmann distribution function in the classical limit actually) or $|C_n|^2 \sim \frac{1}{e^{-\beta E_n} \pm 1}$ in the quantum limit where ± signs are for two different types of particles in the quantum limits called fermions (like electrons, protons etc which has half-integer spins) and bosons (like photon, phonon with integer spins), respectively. We will make this distinction in QM-II course.

- Returning back to our Hilbert space discussion, we have so far discussed about an abstract energy eigenvectors. The Hamiltonian is defined in the phase space of position and momentum. So, we need to obtain results in our physical domain. The advantage of working in the abstract domain (which we will eventually convert into matrix algebra for real computations) is that the results are unique and we can now project the results into any of our favourite domain (either position or momentum or anything else). The way to do that is to define a Hilbert space for the specific domain. Let's say x is the value of the position in the spatial domain and then there is an operator $\hat{x}$ whose eigenvalue is x and eigenket is $|x\rangle$, as defined to be

$$\hat{x}|x\rangle = x|\hat{x}\rangle \qquad \cdots (15)$$

The $|x\rangle$ states also form a Hilbert space since $\hat{x}$ is a linear, Hermitian operator, but here $|x\rangle$ states are continuous and ranges from $|-\infty\rangle$ to $|\infty\rangle$. The states are orthonormalized as $\langle x|x'\rangle = \delta(x-x')$ and the closure/resolution relation is $\int_{-\infty}^{\infty} dx\, |x\rangle\langle x| = 1$.

Now, we can project any abstract ket state into the position domain to obtain a function $\psi(x) = \langle x|\psi\rangle$ which gives a mapping from the domain space to a functional space. In fact, instead of choosing the energy eigenstate's Hilbert space to expand $|\psi\rangle$, one can choose the position space to expand the general state of the particle as

$$|\psi\rangle = \int_{-\infty}^{\infty} dx \;\; c(x) \;\; |x\rangle \qquad --\,(16)$$

Note that eq(16) is actually same as eq(14) in which $\sum_n \to \int dx$ and $c_n \to c(x)$. In fact $c(x) \equiv \psi(x) = \langle x|\psi_n\rangle$. Therefore, the wave function we have defined in the previous chapter is nothing but the probability amplitude of the particle to be at the $|x\rangle$ state, i.e., at position x. The two conditions we did for the discrete energy eigenstate becomes now

(i) $\sum_n |c_n|^2 = \sum_n c_n^* c_n = 1 \quad \Rightarrow \quad \int_{-\infty}^{\infty} dx \;\; \psi^*(x)\,\psi(x) = 1.$

(ii) $\sum_n |c_n|^2 E_n = E \quad \Rightarrow \quad E = \langle\psi|\,\hat{H}\,|\psi\rangle$

$\mathbb{I} = \int dx\, |x\rangle\langle x|$

$\mathbb{I} = \int dx\, |x\rangle\langle x|$

$$= \int_{-\infty}^{\infty} dx\, dx' \; \langle\psi|x\rangle \langle x|H|x'\rangle \langle x'|\psi\rangle$$

$$= \int_{-\infty}^{\infty} dx \;\; \psi^*(x) \; H(x) \; \psi(x)$$

where we have used the fact that the Hamiltonian is defined locally, i.e. $\langle x|\hat{H}|x'\rangle = H(x)\,\delta(x-x')$.

Conditions (i) & (ii) are the two important definitions we have been using for the normalization of the wavefunction and the expectation value of a quantum operator in the previous chapters.

One can also expand each of the energy eigenkets $|\psi_n\rangle$ in the position Hilbert space in the same ways $|\psi_n\rangle = \int_{-\infty}^{\infty} dx\, \psi_n(x)\, |x\rangle$. Then the normalization condition of the energy's Hilbert space becomes $\int_{-\infty}^{\infty} dx\, \psi_m^*(x)\, \psi_n(x) = \delta_{nm}$. Similarly, the abstract eigenvalue equation $\hat{H}|\psi_n\rangle = E_n|\psi_n\rangle$ becomes

$$\langle x|\hat{H}|\psi_n\rangle = \langle x|E_n|\psi_n\rangle$$

$$\Rightarrow \int_{-\infty}^{\infty} dx' \underbrace{\langle x|\hat{H}|x'\rangle}_{H(x)\,\delta(x-x')} \langle x'|\psi_n\rangle = E_n \langle x|\psi_n\rangle.$$

$$\Rightarrow \boxed{H(x)\,\psi_n(x) = E_n\,\psi_n(x)}.$$

This is also the eigenvalue equation in the position space that we have used before.

[The above projection of a Hilbert space into the position Hilbert space can simply be generalized to projection of a Hilbert space into another Hilbert space (like a projecting the Hilbert space of a particle in a box into the Hilbert space of the simple Harmonic oscillators). Lets say we have two discrete Hilbert spaces $\psi_n \in \mathcal{H}_1$ of dim N, $\phi_m \in \mathcal{H}_2$ of dim m. Then for each n^{th} component of ψ_n: $|\psi_n\rangle = \sum_{m=1}^{M} \langle\phi_m|\psi_n\rangle |\phi_m\rangle$, where $\langle\phi_m|\psi_n\rangle = \psi_n(\phi_m) \equiv \psi_{nm}$ is the analog of wavefunction in the ϕ-space.]

- **Momentum's Hilbert space:** The momentum space Hilbert space can be defined similarly : $\hat{p}\,|p\rangle = p\,|p\rangle$, with $\langle p|p'\rangle = \delta(p-p')$ and $\int_{-\infty}^{\infty} \frac{dp}{2\pi}\, |p\rangle\langle p| = 1$. This is also a continuous, infinite dimensional Hilbert space unless some constraint is imposed. For examples, for a particle in a box we have discrete momentum values, or for a periodic lattice, p is periodic outside $0 < p < 2\pi$ (for unit length).

As we expand a momentum state $|p\rangle$ in the Hilbert space of the position operator, we have the expansion coefficients, which we call wavefunction, as $\langle x|p\rangle = e^{ipx}$. These are the plane wave states that we defined in previous chapters. Instead of deriving it, we can verify this relation from the Fourier transformation relation.

As any general state $|\psi\rangle$ is expanded in the position and momentum Hilbert space we have

$$|\psi\rangle = \int dx\ \psi(x)\ |x\rangle = \int \frac{dp}{(2\pi)}\ \psi(p)\ |p\rangle . \quad \text{--- (17)}$$

Multiplying with $\langle x'|$ from the left we get

$$\int dx\ \ \psi(x)\ \underbrace{\langle x'|x\rangle}_{\delta(x-x')} = \int \frac{dp}{(2\pi)}\ \psi(p)\ \underbrace{\langle x'|p\rangle}_{e^{ipx}}$$

$$\Rightarrow \qquad \psi(x') = \int \frac{dp}{(2\pi)}\ \psi(p)\ e^{ipx}.$$

which is the Fourier transformation expression. $\psi(x)$ & $\psi(p)$ are the wavefunctions in the position and momentum space. They are different functions actually and typically denoted by $\psi(x)$, $\tilde{\psi}(p)$ or $\phi(p)$ etc.

• What Hilbert space to use for the general state $|\Psi\rangle$.

By now we have seen atleast four Hilbert spaces (energy, planewave, position and momentum), and clearly there are many more Hermitian operators possible for a given system (such as angular momentum, angle operators, etc etc). If we have two operators commute, then its even better, because the both operators then share the same Hilbert space.

If we add a particle into the system defined by a Hamiltonian with a given energy E, then the particle assumes a state vector $|\Psi\rangle$. To evaluate $|\Psi\rangle$, its always a good idea to expand $|\Psi\rangle$ in any of the Hilbert space specific to the system, ie, the Hamiltonian. Obviously, the most convenient Hilbert space is the energy eigenstates Hilbert space $H|\Psi_n\rangle = E_n|\Psi_n\rangle$. If the Hamiltonian commutes with some operator(s), then the energy eigenstates are also eigenstates of that operator. For example, if linear momentum is conserved, then momentum operator commutes with the Hamiltonian (to be derived below), or if the angular momentum is conserved for rotations mainly, then the angular momentum L commutes with the Hamiltonian. Then the energy eigenstates $|\Psi_n\rangle$ are also eigenstates of those conserved operators, $\hat{p}\,|\Psi_n\rangle = \hbar k\,|\Psi_n\rangle$

or $\hat{L}|\psi_n\rangle = l\hbar|\psi_n\rangle$. In such cases, the eigenkets can also be indexed by k or l, as appropriate, as $|\psi_{n,k}\rangle$ or $|\psi_{n,l}\rangle$. We will see examples of those later.

But we may not be always lucky to solve the entire Hamiltonian to obtain the energy eigenstates, especially for complicated potential. How would you, in general, approach it?

We will look at the Hamiltonian and try to find out first if is any conserved operator, like momentum / angular momentum etc. If there is one or more, we are essentially done. We can use its Hilbert space to obtain the Hilbert space of the Hamiltonian.

But if this is not the case, we will look into parts of the Hamiltonian, say, kinetic energy part, or potential energy, or if the Hamiltonian involves angular momentum operator etc. Then we will start with the Hilbert space of such an operator. In this way, atleast, some part of the Hamiltonian is solved and we will proceed to solve the remaining part accordingly. Let us think of the generic case of $\hat{H} = \hat{K} + \hat{V}$. Typically, the kinetic energy operator $\hat{K}$ is a function of momentum operator. Hence we can use the momentum space Hilbert space $|p\rangle$: $\hat{K}(\hat{p})\,|p\rangle = K(p)\,|p\rangle$, where $K(p)$ is the eigenvalue of the $\hat{K}$ operator in this Hilbert space. ☺

But potential energy operator is typically a function of position operator $\hat{V}(\hat{x})$. Therefore, the momentum states $|p\rangle$ are the worst state for the potential energy, because $|p\rangle$ is not an eigenstate of the position operator $\hat{x}$. This is because of the uncertainty principles between position and momentum. We will show below that the uncertainty between two variable is related to the fact that the corresponding to operators do not commute. Since they donot commute, they do not share the same eigenstates. So, the eigenstates of the momentum operator is not an eigenstate of the position operator. In fact $|p\rangle$ is the worst state for the position operator, because $|p\rangle$ is the eigenstate of p which thus have no uncertainty $\Delta p = 0$. This makes the uncertainty of position in this $|p\rangle$ states the maximum as $\Delta x \geq \frac{h}{2\Delta p}$.

For the same reason, the position states $|x\rangle$ are the eigenstates of the potential energy, but its the worst state, with maximum uncertainty for the momentum and hence the kinetic energy operator.

Note that the momentum states becomes the plane wave state when projected on to the position space as $\langle x|p\rangle = e^{ipx}$, which we found to be the eigenstates of free particles, i.e., no potential energy and only kinetic energy. This is in consistent with what we just said above: The momentum of a plane wave (ie, its wave length) is completely known, but its position is completely unknown since the particle is always oscillating in space.

On the other hand, the position states $|x\rangle$ becomes the delta-function when projected on to the position space itself, because of the normalization condition $\langle x'|x\rangle = \delta(x'-x)$. The delta function wavefunction means the particle is completely localized and it has no momentum, i.e. no kinetic energy. So, momentum uncertainty is infinity. Therefore, the potential energy tries to localize the wavefunction, while the K.E. tries to delocalize them – an interpretation which also hold in the classical Mechanics.

What we did earlier is that we rather constructed something in between the two – called the wavepackets which are like damped/decaying oscillation. The decay length of the wavepacket (typically the classical turning point) such that it has the least uncertainty with momentum (wave vector/wavelength inverse of the oscillatory path. This way the wavepacket are designed to follow $\Delta p \Delta x = \hbar/2$ relation, and hence gives the least uncertainty. When the wave packets become the eigenstate of the Hamiltonian with discrete eigen energies, they form a Hilbert space.

Apart from the position, momentum operators, the other operators we often look at is the angular momentum operator, usually for spherically symmetric case. The above story then repeats between angular momentum operator/eigenstates versus rotation angle operator $\hat{\Theta}$ and its Hilbert space. We will see one example for the Hydrogen atom case.

(***) Relation between Commutator and Heisenberg uncertainty principle.

We have mainly used uncertainty relation between position & momentum $\Delta x \Delta p \geq h/2$ (or between the phase space variables. We have also seen/discuss that $\hat{x}, \hat{p}$ operators do not commute and we have $[\hat{x}, \hat{p}] = i\hbar$ [inheriting the Poisson bracket relation in classical mechanics $\{x, p\} = 1$]. Our job is to connect these two relations as $\langle \Delta x\rangle \langle \Delta p\rangle \geq -i\langle[\hat{x}, \hat{p}]\rangle$ where the expectation values are obtained in any general Hilbert space. The uncertainty value depends on in which Hilbert space the expectation values are computed. If there is a Hilbert space which gives $\langle \Delta x\rangle\langle \Delta p\rangle = \hbar/2$, then this is the least uncertainty possible. That the wavepacket state. Such least uncertainty states are called coherent states. This relation is actually much more general and fundamental to any two linear, Hermitian operators $\hat{A}$ & $\hat{B}$ which do not commute. So, we start with such a general case first. It is easy to show that the commutator $[\hat{A}, \hat{B}]$, which is also an operator, is an anti-Hermitian operator, for $\hat{A}$ & $\hat{B}$ two Hermitian operator. Writing an anti Hermitian operator in terms of 'i' times a Hermitian operator ($\hat{D}$) we have our starting point

$$[\hat{A}, \hat{B}] = i\hat{D} \quad \cdots \quad (18)$$

- We also need to understand whats the definition of variance/uncertainty. In the probability theory, this is called the 2nd moment of an observable which measures the square of the variation of the observable from its average/expectation value. Lets say, we are making the measurements of the $\hat{A}$ operator in the general state vector of the particle $|\psi\rangle$, with the average value is $\langle \hat{A}\rangle = \langle\psi|\hat{A}|\psi\rangle$. Then we define an operator $\bar{A}$ which measures the deviation of the result from its mean value as $\bar{A} = A - \langle A\rangle$. Then the variance/uncertainty is defined as

$$(\Delta A)^2 = \langle\psi|\bar{A}^2|\psi\rangle = \langle\bar{A}^2\rangle$$
$$= \langle (A-\langle A\rangle)(A-\langle A\rangle)\rangle = \langle A^2\rangle - \langle A\rangle^2 \quad \text{---(19).}$$

Similarly, $(\Delta B)^2 = \langle\bar{B}^2\rangle = \langle B^2\rangle - \langle B\rangle^2$, where $\bar{B} = B - \langle B\rangle$.

Notice that $[\bar{A}, \bar{B}] = [A, B] = iD$ ---(20).

- We want to prove that $(\Delta A)(\Delta B) \geq \frac{1}{2}|\langle [A,B]\rangle|$, ---(21).

which is same as $\langle\bar{A}^2\rangle\langle\bar{B}^2\rangle \geq \frac{1}{4}|\langle[\bar{A},\bar{B}]\rangle|^2$ ---(22)

where we have squared both sides of eq(21) for convenience.

- $\langle\bar{A}^2\rangle = \langle\underbrace{\psi|\bar{A}}\,\underbrace{\bar{A}|\psi}\rangle = \langle\bar{A}\psi|\bar{A}\psi\rangle$ Since $\bar{A}$ is Hermitian.

We call it a state $|\psi_a\rangle = |\bar{A}\psi\rangle$. Similarly $\psi_b = |\bar{B}\psi\rangle$.

Then the L.H.S of eq(22) is $\langle\psi_a|\psi_a\rangle\langle\psi_b|\psi_b\rangle$. Lets now use the Schwartz inequality

$$\langle\psi_a|\psi_a\rangle\langle\psi_b|\psi_b\rangle \geq |\langle\psi_a|\psi_b\rangle|^2, \quad \text{---(23).}$$

where $\langle \psi_a | \psi_b \rangle = \langle \psi | \bar{A}\bar{B} | \psi \rangle$ = a complex number $= z$. We now need to convert the R.H.S to the commutator for which looks like $z - z^* = \langle \psi | \bar{A}\bar{B} - \bar{B}\bar{A} | \psi \rangle = \frac{1}{2i} \mathrm{Im}(z)$. Of course, $|z|^2 \geqslant (\mathrm{Im}(z))^2$. Therefore, $|\langle \bar{A}\bar{B} \rangle|^2 \geqslant \frac{1}{4} |\langle [\bar{A}, \bar{B}] \rangle|^2$. Substituting this in eq (22), we get

$$\boxed{\langle \bar{A}^2 \rangle \langle \bar{B}^2 \rangle \geqslant \frac{1}{4} |\langle [\bar{A}, \bar{B}] \rangle|^2}.$$

- H.W. In eq (18), R.H.S we have a Hermitian operator $\hat{D}$. If we choose its eigenstates $\hat{D}|d\rangle = d|d\rangle$, where d is real, in the Hilbert space we have $\langle [A, B] \rangle = i d$. Then we can show that $\Delta A \, \Delta B \geqslant d/2$ where the variances ΔA, ΔB are for a measurement in any general state. Is it true that the least uncertainty is obtained in the Hilbert space of $\hat{D}$? I have not checked it.

- So, the conclusion is that if two linear, Hermitian operators do not commute, then they cannot be simultaneously measured with arbitrary precision.
- But if they commute, then they share the same eigenstates and hence in that eigenstate, the variances of both operators are completely zero.

- For, $\hat{A} = \hat{x}$, $\hat{B} = \hat{p}$, we have $[\hat{x}, \hat{p}] = i\hbar$. Then we obtain the uncertainty relation $\Delta x \, \Delta p \geqslant \hbar/2$.

A wavepacket (or a coherent state) is a state which gives the least uncertainty $\Delta x \, \Delta p = \hbar/2$. Therefore, if Δx is the variance of the wavefunction in position space, it should roughly look like $\psi(x) \sim C \exp\left[-\frac{(x - \langle x \rangle)^2}{\Delta x}\right]$. The momentum space wavefunction would then look like

$$\psi(p) = D \exp\left[-\frac{(p - \langle p \rangle)^2}{\Delta p}\right] = D \exp\left[\frac{-2(p - \langle p \rangle)^2 \Delta x}{\hbar}\right].$$

Plugging them into the Fourier transformation we get

$$\psi(x) = D \int dp \, \exp\left[\frac{-2(p - \langle p \rangle)^2 \Delta x}{\hbar}\right] \exp(ipx).$$

$$\sim D \exp\left[i \langle p \rangle x\right] \exp\left[-\frac{(\Delta p)^2 (x - \langle x \rangle)^2}{\hbar^2}\right]. \quad \text{-- (24)}$$

Matrix Representation of state vector & operators

All the mathematical formulations we have carried out above for the 'ket', 'bra' state vectors, operators, eigenvalue equation are very similar or even same to the matrix algebra. The connection between the abstract linear algebra and the linear matrix Algebra is as follows : A ket vector $|\psi\rangle$ becomes a column vector, its dual 'bra' vector $\langle\psi|$ becomes a row vector with the complex conjugation of all components (essentially the Hermitian conjugate '$\dagger$' operation we define in matrix algebra), an operator becomes a (square) matrix, while the inner product and expectative values becomes scalar numbers. The dimension of the vectors / matrices are not fixed, and it depends on the Hilbert space dimension. The Hilbert space becomes a set of linearly independent, normalized (unit) column vectors of dimension N where N is the Hilbert space. A simple example would be for a Hilbert space of $|\psi_n\rangle \in \mathcal{H}_N$, we can have -

$$|\psi_1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ \vdots \end{pmatrix}_{N\times 1}, \quad |\psi_2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ \vdots \end{pmatrix}_{N\times 1}, \quad |\psi_3\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ \vdots \end{pmatrix}_{N\times 1}, \quad \cdots\cdots, \quad |\psi_N\rangle = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ 0 \\ 1 \end{pmatrix}_{N\times 1}.$$

and the dual space is $\langle\psi_1| = \begin{pmatrix} 1 & 0 & 0 & \cdots \end{pmatrix}_{1\times N}, \;\cdots,\; \langle\psi_N| = \begin{pmatrix} 0 & 0 & \cdots & 1 \end{pmatrix}_{1\times N}$

(We keep denoting the column vectors by $|\psi\rangle$ although its not a standard notation)

- The normalization is defined by $\langle \psi_n | \psi_n \rangle = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 1 \\ 0 \\ \vdots \end{pmatrix}^{\dagger} \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ \vdots \end{pmatrix}$

$$= \begin{pmatrix} 0 & 0 & \cdots & 1 & 0 & \cdots \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 1 \\ 0 \\ \vdots \end{pmatrix} = 1.$$

- Its also easy to see that these unit vectors are orthogonal $\langle \psi_n | \psi_m \rangle = \delta_{nm}$.
- They also follow the closure relation (outer product)

$$\sum_{n=1}^{N} |\psi_n\rangle\langle\psi_n| = \begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \end{pmatrix} \begin{pmatrix} 1 & 0 & \cdots \end{pmatrix} + \begin{pmatrix} 0 \\ 1 \\ 0 \\ \vdots \\ \vdots \end{pmatrix} \begin{pmatrix} 0 & 1 & 0 & \cdots \end{pmatrix} + \cdots + \begin{pmatrix} 0 \\ 0 \\ \vdots \\ \vdots \\ 1 \end{pmatrix} \begin{pmatrix} 0 & \cdots & 1 \end{pmatrix}$$

$$= \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & 0 \\ \vdots & \vdots & \vdots & & \ddots \\ 0 & 0 & 0 & \cdots 0 & 1 \end{pmatrix} = \mathbb{I}_{N\times N} \text{ (unit matrix)}$$

- Therefore, any arbitrary column vector can be expanded in this unit vector space (~ Hilbert space although one does not call it a Hilbert space in the matrix algebra language).

$$|\psi\rangle = \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ \vdots \\ c_n \end{pmatrix} \Rightarrow |\psi\rangle = c_1 \begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \end{pmatrix} + c_2 \begin{pmatrix} 0 \\ 1 \\ 0 \\ \vdots \end{pmatrix} + \cdots + c_N \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 1 \end{pmatrix} \quad \text{---} (1)$$

$$= \sum_n c_n |\psi_n\rangle, \text{ where } c_n = \langle \psi_n | \psi \rangle$$

- An operator $\hat{A}$ is a $N \times N$ matrix in a unit vector space of dimension N and its components are a_{nm}.

$$A = \begin{pmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1N} \\ a_{21} & a_{22} & a_{23} & \cdots & a_{2N} \\ a_{31} & a_{32} & a_{33} & \cdots & a_{3N} \\ \vdots & \vdots & \vdots & \ddots & \\ a_{N1} & a_{N2} & a_{N3} & & a_{NN} \end{pmatrix}$$

A Hermitian matrix means $A^{+} = A \Rightarrow (a_{nm})^{*} = a_{mn}$.

where the Hermitian conjugate $+$ means complex conjugation + transpose.

- Expectation value of this operator is defined as

$$\langle A \rangle = \langle \psi | A | \psi \rangle = \begin{pmatrix} c_1^{*} & c_2^{*} & \cdots & c_N^{*} \end{pmatrix} \begin{pmatrix} a_{11} & a_{12} & & \\ a_{21} & a_{22} & & \\ \vdots & & \ddots & \\ & & & a_{NN} \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_N \end{pmatrix}$$

$$= \begin{pmatrix} c_1^{*} & c_2^{*} & \cdots & c_N^{*} \end{pmatrix}_{N \times 1} \begin{pmatrix} a_{11} c_1 + a_{12} c_2 \cdots c_{1N} c_N \\ \vdots \\ \vdots \end{pmatrix}_{1 \times N}$$

$$= c_1^{*} (a_{11} c_1 + a_{12} c_2 \cdots a_{1N} c_N) + c_2^{*} (\qquad) + \cdots$$

$$= \sum_{m,n} c_n^{*} a_{nm} c_m \qquad \cdots (2)$$

- Eigenvalue and eigenvector of a matrix operator

If $|\psi\rangle$ is an eigenvector of a matrix A, with eigenvalue '$\hat{a}$', then $\hat{A}|\psi\rangle = a|\psi\rangle$, where A is a N×N matrix, $|\psi\rangle$ is a 1×N column vector and a is a scalar number. '$\hat{a}$' is real if A is Hermitian. For a N×N matrix, there are N eigenvalues (including any degeneracy) which we index as a_n, and for each eigenvalue there is a corresponding eigenvector $|\psi_a\rangle$. It can be shown that all the 1×N eigenvectors are linearly independent, can be normalized to unity, and follow the closure property. Therefore, they form a Hilbert space analog of complete set of N-component basis vectors. Any general, normalizable, N-component column vector can be expanded in this basis unit vectors as eq(1).

Using all the eigenvectors, we can construct a unit matrix by arranging them into different column as

$$U = \begin{pmatrix} |\psi_1\rangle & |\psi_2\rangle & \cdots & |\psi_N\rangle \\ \vdots & \vdots & & \vdots \\ \vdots & \vdots & & \vdots \end{pmatrix}$$

which is a N×N unitary matrix, $U^{+} = U^{-1}$ & $U^{+}U = I$. This is the particular unitary rotation/transformation to the matrix A which diagonalized it. In mathematical form it reads $UAU^{+} = D$ where D is a diagonal matrix with the eigenvalues a_n are in its diagonal positions.

- The unitary transformations are defined as in the abstract linear algebra : Matrix : $A \to A' = UAU^{+}$.

  Vector : $|\psi\rangle \to |\psi'\rangle = U|\psi\rangle$

  Scalar : $a \to a' = UaU^{+} = a$

  The inner product / normalization, eigenvalue equation and expectation values are invariant under unitary transformations as in the Linear Algebra case. Therefore, symmetry operations are denoted by unitary transformation.

- The trace of an operator is defined by introducing a complete orthonormal set of basis vectors as

  $$\mathrm{Tr}A = \sum_n \langle\psi_n|A|\psi_n\rangle = \sum_n a_n = \text{Sum over eigenvalues.}$$

  This definition is useful because the trace, where it exists, is independent of the choice of basis vectors.

- This gives a brief but comprehensive introduction to the matrix algebra to show that the quantum mechanics can be formulated as well by matrix algebra. This was done independently by Heisenberg and Dirac.

- Continuous Hilbert space to matrix formulation

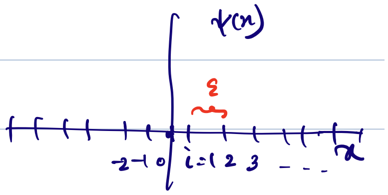
The continuous Hilbert space that we defined for the position, momentum space in the linear Algebra case are rather harder to find exact analog in the vector / matrix algebra. But for practical computations, especially in numerical simmulation, one would discritize the continuous variable and then define a matrix. We will see one example below.

e.g. Schrödinger equation in continuous position space to matrix formulation

(This is not a part of QM-I course, but I have added it just to get a feel of how one solves a Schrödinger equation on a computer).

We start with the schrödinger equation in one space dimension

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + V(x)\,\psi(x) = E\,\psi(x). \quad \text{- - - (a)}$$



We see that all terms are local, and defined at a given position, except the first term. This term is actually a second order differential equation. We use the definition of the derivative as

$$\frac{d\psi}{dx} = \lim_{\varepsilon\to 0}\frac{\psi(x+\varepsilon)-\psi(x)}{\varepsilon},$$

$$\frac{d^2\psi}{dx^2} = \lim_{\varepsilon\to 0}\frac{\frac{\psi(x+\varepsilon)-\psi(x)}{\varepsilon} - \frac{\psi(x)-\psi(x-\varepsilon)}{\varepsilon}}{\varepsilon} = \lim_{\varepsilon\to 0}\frac{\psi(x+\varepsilon)+\psi(x-\varepsilon)-2\psi(x)}{\varepsilon^2}.$$

Therefore, we can discretize the space into small bin of width $\varepsilon \to 0$ and denote those discrete positions by x_i, where $i \in$ integer running from $-\infty$ to ∞. Each position x_i is an eigenvalue of the discrete Hilbert space now $\hat{x}|x_i\rangle = x_i|x_i\rangle$. At each position, we project the state vector $|\psi\rangle$ to define $\psi(x_i) = \langle x_i|\psi\rangle = \psi_i$. Starting with some position x_i, the 2nd derivative term then reads as

$$\frac{d^2\psi}{dx^2} = \lim_{\varepsilon \to 0} \frac{1}{\varepsilon^2}\left(\psi_{i+1} + \psi_{i-1} - 2\psi_i\right). \quad \text{-- (2)}$$

Then from the schrödinger equation we have

$$-\frac{\hbar^2}{2m\varepsilon^2}\left(\psi_{i+1} + \psi_{i-1} - 2\psi_i\right) + V_i\,\psi_i = E\,\psi_i \quad \text{-- (3)}.$$

This equation can be converted into a matrix equation by defining a state column vector

$$\underline{\Psi} = \begin{pmatrix} \vdots \\ \psi_{i-1} \\ \psi_i \\ \psi_{i+1} \\ \vdots \end{pmatrix}$$

Then eqn(3) can be written as

$$\underbrace{\begin{array}{c}\begin{pmatrix} \ddots & 0 & 0 & 0 & 0 & \\ 0 & \frac{\hbar^2}{m}+V_i & -\frac{\hbar^2}{2m} & 0 & 0 & \\ 0 & -\frac{\hbar^2}{2m} & \frac{\hbar^2}{m}+V_{i-1} & -\frac{\hbar^2}{2m} & 0 & 0 \\ 0 & 0 & -\frac{\hbar^2}{2m} & \frac{\hbar^2}{m}+V_i & -\frac{\hbar^2}{2m} & 0 \\ 0 & 0 & 0 & -\frac{\hbar^2}{2m} & \frac{\hbar^2}{m}+V_{i+1} & 0 \\ 0 & 0 & 0 & 0 & 0 & \ddots \end{pmatrix} \\ \begin{array}{cccccc} \quad & \quad & i-1 & i & i+1 & \quad \end{array}\end{array}}_{H} \underbrace{\begin{pmatrix} \vdots \\ \psi_{i-1} \\ \psi_i \\ \psi_{i+1} \\ \vdots \end{pmatrix}}_{\Psi} = \underbrace{E}_{E} \underbrace{\begin{pmatrix} \vdots \\ \psi_{i-1} \\ \psi_i \\ \psi_{i+1} \\ \vdots \end{pmatrix}}_{\Psi}.$$

This way we converted our schrödinger equation in continuous space to a matrix formulation $\hat{H}\psi = E\psi$. We can solve it on a computer or we can do a discrete Fourier transformation. We will not solve it here though. This is clearly an approximate method since the accuracy increases with reducing ε. For numerical method we also have to truncate it at some finite size system or one takes a periodic boundary condition.

⊛ Schrödinger vs Heisenberg formulation

- Schrödinger proposed the famous Schrödinger equation of motion for continuous variables (x, p) and a continuous function $\psi(x)$ which takes the shape of a (discrete) eigenvalue and eigenfunction format when we enforce normalizability condition on the wavefunction and certain boundary conditions.
- Heisenberg independently also proposed a matrix formulation of the quantum mechanics, mainly for discrete basis such as spin etc. His approach was more of taking Hamiltonian formalism in the classical mechanics and making them as operators. In his way of constructing quantum mechanics from classical mechanis (which was later also expanded by Dirac) is as follows:

Classical Mechanics		Quantum Mechanics
• Variables: $\vec{r}, \vec{p}, \theta, \vec{L}, E$	→	Operators $\hat{\vec{r}}, \hat{\vec{p}}, \hat{\theta}, \hat{\vec{L}}, \hat{H}, \ldots$
• Time (t) is not a degree of freedom, rather it governs the dynamics to the degrees of freedom.	→	So time is also not an operator in a strict sense, but a variable.
• Dynamics is defined in phase space of $(\vec{r}, \vec{p}), (\theta, L), \ldots$	→	We have Hilbert space, made of eigenvectors of operators.

- Dynamics in the phase is restricted by Poisson bracket $\{x, p_x\}_{P.B.} = 1, \dots$ → Dynamics in QM is restricted by commutator $[x, p_x] = i\hbar$, leading to uncertainty principle. (Energy time uncertainty has no commutator)

- Time evolution is governed by Hamilton's principles. → Time evolution of an operator is governed by Heisenberg relation (to be derived below)

$$\dot{x} = \frac{\partial H}{\partial p}, \quad \dot{p} = -\frac{\partial x}{\partial x}$$

and more generally for a variable A:

$$\frac{dA}{dt} = \{A, H\}_{P.B.} + \frac{\partial A}{\partial t}.$$

$$\frac{d\hat{A}}{dt} = \frac{i}{\hbar}[\hat{H}, \hat{A}] + \frac{\partial \hat{A}}{\partial t}.$$

(Or, time evolution of the wave function / Hilbert space is determined by the time-dependent Schrödinger equation

$$i\hbar \frac{\partial}{\partial t}\Psi(t) = \hat{H}\Psi(t).)$$

(Conserved quantity A are denoted by $\{A, H\}_{P.B.} = 0$)

(Conserved operator $\hat{A}$ is denoted by $[\hat{H}, \hat{A}] = 0$.)

(Caution: The dictionary / analogy between classical variable to quantum operator is a hyphoses / observation of Dirac, and there is no rigourous proof or theorem to justify that. Bohr's correspondence principicle is also a hypothesis that any quantum mechanical equation should reproduce the classical equation as $h \to 0$. This is what the expectation values of operator does according to the Ehrenfest's theorem, to be seen below).

- Time evolution :

We briefly discuss the time dependence of the system in the abstract state vector and operator language. We start with the time-dependent Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = \hat{H} |\psi(t)\rangle \quad --(1)$$

This is an abstract operator equation which can be converted into our familiar Schrodinger equation by projecting onto the position space $\langle x|$. We will continue with abstract space here.

Eq (1) points the direction of the state vector $|\psi(t)\rangle$ at all points in space (ie, eq(1) is local in space). We have discussed its solution earlier, that the solution with respect to the boundary condition that at initial time $t_0=0$, $|\psi(t)\rangle = |\psi(0)\rangle$ and H is here assumed to be time-independent. This gives

$$|\psi(t)\rangle = \hat{U}(t)\,|\psi(0)\rangle = e^{-i\hat{H}t/\hbar}\,|\psi(0)\rangle \quad --(2)$$

where $\hat{U}(t) = e^{-i\hat{H}t/\hbar}$ is the unitary operator which make sure the states inner product is time-independent, ie, $\langle\psi(0)|\psi(0)\rangle = \langle\psi(t)|\psi(t)\rangle$.

The expectation value of an operator A at time t is

$\langle A\rangle_t = \langle\psi(t)|\,\hat{A}\,|\psi(t)\rangle$, where we have assumed the operator $\hat{A}$ has no explicit time dependence, ie $\frac{\partial \hat{A}}{\partial t} = 0$, but $\frac{d\hat{A}}{dt}$ may not be zero. (Think of $\hat{A}$ as $\hat{x}, \hat{p}, \hat{H}$ etc as example). Then we write

$$\begin{aligned} \langle A \rangle_t &= \langle \psi(t) | \hat{A} | \psi(t) \rangle \\ &= \langle e^{-iHt/\hbar} \psi(0) | \hat{A} | e^{-iHt/\hbar} \psi(0) \rangle \\ &= \langle \psi(0) | \underbrace{\underbrace{e^{iHt/\hbar}}_{U^{+}} \hat{A} \underbrace{e^{-iHt/\hbar}}_{U.}}_{\hat{A}(t).} | \psi(0) \rangle \\ &= \langle \psi(0) | \hat{A}(t) | \psi(0) \rangle . \qquad -- (3). \end{aligned}$$

We see a wonderful relation that it does not matter where the time evolution is implemented with the state vector $|\psi(t)\rangle$ while keeping $\hat{A}$ time independent, or the state vector is kept time-independent $|\psi(0)\rangle$ and the operator is evolved in time $\hat{A}(t)$. The expectation values don't change and, of course, the state vectors normalization also don't change. This was the property of the unitary property of the time evolution operator which stems from the Hermitian property of the Hamiltonian operator. The former procedure is called the Schrödinger picture while the later procedure is called the Heisenberg picture. More about it will be taught in QM-II course.

- Lets proceed with studying the dynamics of $\hat{A}(t)$. We obtain

$$\frac{d\hat{A}(t)}{dt} = \frac{d}{dt}\left(e^{i\hat{H}t/\hbar}\,\hat{A}(0)\,e^{-i\hat{H}t/\hbar}\right)$$

since $\hat{H}$ commutes with itself

$$= \frac{i\hat{H}}{\hbar}\, e^{iHt/\hbar}\,\hat{A}(0)\,e^{-i\hat{H}t/\hbar} + e^{iHt/\hbar}\,\frac{\partial\hat{A}}{\partial t}(0)\,e^{-iHt/\hbar} + e^{iHt/\hbar}\,\hat{A}(0)\left(-\frac{i\hat{H}}{\hbar}\right)e^{-iHt/\hbar}.$$

$$= \frac{i}{\hbar}\, e^{iHt/\hbar}\left(\hat{H}\hat{A}(0) - \hat{A}(0)\hat{H}\right)e^{-iHt/\hbar} + e^{iHt/\hbar}\,\frac{\partial\hat{A}}{\partial t}(0)\,e^{-iAt/\hbar}.$$

This is to say the partial derivative of $\hat{A}$ at $t=0$.

$$= \frac{i}{\hbar}\left[\hat{H}(t),\hat{A}(t)\right] + \left(\frac{\partial\hat{A}}{\partial t}\right)(t)$$

(First partial derivative is done at $t=0$, and then it is evolved in time).

$$\Rightarrow \boxed{\frac{\partial\hat{A}(t)}{\partial t} = \frac{i}{\hbar}\left[\hat{H}(t),\hat{A}(t)\right] + \frac{\partial\hat{A}}{\partial t}} \quad ---(1)$$

This is the Heisenberg's equation of time evolution of the system if the time evolution is embedded in the operator and not in the state. Otherwise, in the schrödinger picture, we have the time-dependent schrödinger eq(1) for the time evolution of the state & operator is time-independent. Both are equivalent.

- If an operator commutes with the Hamiltonian and that this operator has no explicit time-dependence, then this operator and its eigenvalues are conserved, i.e., time-independent.

  Hamiltonian commutes with itself, so Hamiltonian and energy are always consered.

  Since conserved operator means it commutes with the Hamiltonian, so they share the same eigenfunctions. Therefore, energy eigenstates can be indexed with the eigenvalues of the conserved operators. They are called quantum numbers.

- H.W. Using Heisenberg picture, show that $\frac{d\hat{x}(t)}{dt} = \frac{i}{\hbar}[\hat{H}(t), \hat{x}(t)]$ and $\frac{d\hat{p}(t)}{dt} = \frac{i}{\hbar}[\hat{H}(t), \hat{p}(t)]$, much like the Hamilton's principles in the classical mechanics.

  [Starting from these relations and using the commutator $[\hat{x}, \hat{p}] = i\hbar$, obtain the Hamilton's principles: $\frac{dx(t)}{dt} = \frac{\partial H(t)}{\partial p(t)}$ and $\frac{dp(t)}{dt} = -\frac{\partial H(t)}{\partial x(t)}$. (Caution: I am not sure if these relations are true ~~for~~ for operators or the expectation values. I have not checked it explicitly, but you have to check it and find out whether the relations hold for the operators $\hat{x}, \hat{p}$ or for the expectation values $\langle\hat{x}\rangle, \langle\hat{p}\rangle$)]

- **Time evolution of the expectation values :**

$$\frac{d}{dt}\langle\hat{A}\rangle = \frac{i}{\hbar}\langle[\hat{H},\hat{A}]\rangle + \left\langle\frac{\partial\hat{A}}{\partial t}\right\rangle . \qquad \cdots (5)$$

where $\frac{d\langle\hat{A}\rangle}{dt} = \frac{d}{dt}\langle\psi|\hat{A}|\psi\rangle$ and $\left\langle\frac{\partial\hat{A}}{\partial t}\right\rangle = \langle\psi|\frac{\partial\hat{A}}{\partial t}|\psi\rangle$..

[H.W. Rederive eq(5) using the schrödinger eq (1).].

- **Ehrenfest's Theorem:** we have derived this theorem before that the center of the wave packet $\langle\vec{r}\rangle$ and its momentum $\langle\vec{p}\rangle$ follows Newtonian equation :

$$\left.\begin{aligned} \frac{d\langle\vec{r}\rangle}{dt} &= \frac{1}{m}\langle\vec{p}\rangle \\ \frac{d\langle\vec{p}\rangle}{dt} &= -\langle\vec{\nabla}V(\vec{r})\rangle \end{aligned}\right\} - (6)$$

We had a long derivation of this theorem before, but now its much easier to do using eq(5) in which we substitute $\hat{H} = \frac{\hat{p}^2}{2m} + \hat{V}(\vec{r})$. The interpretation of eq (6) is that if we take the expectation value of the position and momentum operator w.r.to a wave function $\psi(\vec{r})$, which represents a wavepacket of a particle, then the trajectory of the wavepacket is governed by the Newton's laws in which we can read of the average force on the wavepacket as $\langle \vec{F} \rangle = -\langle \vec{\nabla} V \rangle$, which is equal to the accelération. Remember that Eq 6 is not valid at the operator level, but only for the expectation values.

H.W. Its obvious that one can hence obtain relations like average angular momentum $\langle \vec{L} \rangle$ follows:

$$\frac{d\langle \vec{L} \rangle}{dt} = -\langle \vec{r} \times \vec{p} \rangle = -\langle \vec{r} \times \vec{\nabla} V \rangle = -\langle \vec{r} \times \vec{F} \rangle.$$

- The Virial Theorem: We have used virial expansion in statistical mechanics for a weakly interactions molecules, in which departures from the ideal gas laws can be related to the virial of a particle $-\frac{1}{2}\sum_i \vec{r}_i \cdot \vec{F}$. We can obtain that relation here that

$$\langle \vec{r} \cdot \vec{F} \rangle = -\langle \vec{r} \cdot \vec{\nabla} V \rangle = 2\langle K \rangle \quad -- (7).$$

where K & V are the K.E. & P.E of the Hamiltonian $H = K + V = p^2/2m + V(\vec{r})$. (In classical mechanics the average is taken over a long time which is assumed to be equal to the average taken over ensembles in statistical mechanics - called Ergotic theorem. Here in quantum mechanics, the average in eq(7) is replaced by the expectation value in a Hilbert space.)

The virial relation in eq (7) is a stationary state solution of a time dependent quantity $\langle \vec{r}\cdot\vec{p}\rangle$
We can calculate its time-dependence from eq(5).

$$\frac{d}{dt}\langle \vec{r}\cdot\vec{p}\rangle = \frac{i}{\hbar}\langle[H, \vec{r}\cdot\vec{p}]\rangle .$$

(H.W.). Show that

$$[H, \vec{r}\cdot\vec{p}] = i\hbar\left(\vec{r}\cdot\vec{\nabla}V\right) - 2i\hbar\langle K\rangle$$

This gives $\frac{d}{dt}\langle \vec{r}\cdot\vec{p}\rangle = 2\langle K\rangle - \left(\vec{r}\cdot\vec{\nabla}V\right)$. --- (8).
The stationary state solution of eq(8) yields eq(7).

The virial theorem becomes particularly useful when the potential energy has a power law dependence on the position, typically they are long range interactions, such as Coulomb interaction $V(r) \sim 1/r$, or simple Harmonic oscillator $V(r) \propto r^2$. One useful property of such potential is that they are called homogeneous function. If we strech/contact the position by a constant, say λ as $r \to \lambda r$, then the form of the potential does not change, only a λ comes out from the potential energy as

$$V(\lambda r) = \lambda^D V(r) ,$$ where D is called scaling dimension and depends on the potential energy. The homogeneous potential satisfies the Euler identity $\vec{r}\cdot\vec{\nabla}V = D\,V(\vec{r})$. Then from eq(7) we get $\langle K\rangle = \frac{D}{2}\langle V\rangle$ at the stationary state.

- Continuity equation : (H.W) (i) Derive the continuity equation for the probability density $\rho(\vec{r}) = \langle\psi(\vec{r})|\psi(\vec{r})\rangle$ and probability current $\vec{J}(\vec{r})$ from eq(5).

  (ii) Using continuity equation prove that $\frac{d\langle\vec{r}\rangle}{dt} = \int \vec{J}\, d^3r$.

Operator Approach to Harmonic Oscillator

We have already solved the simple Harmonic oscillator problem by solving 2nd order differential equation and found that the normalizable solutions are those in which the series solutions truncate at finite values. Those series of values give different linearly independent wavefunctions written as a product of Hermite polynomial and a Gaussian wavepacket. The corresponding eigenvalues are $E_n = (n+1/2)\hbar\omega$.

Now we will employ an operator approach - also called the Algebraic approach, to solve the same Hamiltonian. The harmonic oscillator potential is unique in which both momentum & position variables are quadratic.

$$H = \frac{1}{2m}\hat{p}^2 + \frac{1}{2}m\omega^2\hat{x}^2 \qquad \text{where } \omega = \sqrt{\frac{k}{m}}.$$

$$= \frac{1}{2}m\omega^2\left(\frac{\hat{p}^2}{m^2\omega^2} + \hat{x}^2\right). \qquad --(1)$$

This quadratic form of the Hamiltonian makes it possible to write this Hamiltonian in a factorized form $H = \hat{A}^{+}\hat{A}$, where is some non-Hermitian operator that we will build below, $A^{+}A$ is hermitian. This factorized

Hamiltonian gives a very simple and elegant set of solutions. In fact we will see that we only have to solve the ground state wavefunction by solving a first order differential equation and then we can just build all the excited states by simply applying A^+ operator on the ground state. This method is so simple and elegant that in the future (perhaps QM-III or QFT course) we will replace any of our Hamiltonian with a fictitious Hamiltonian of this A^+A form with both having the same set of energy eigenvalues. That is to use the Hilbert space of this operator A^+A and expand any Hamiltonian in this Hilbert space. That procedure is called the Second quantization method. Therefore, the solutions of Harmonic oscillator is going to be useful for our entire life even in advanced research.

Let us factorize the Hamiltonian in eq(1). It has the form a^2+b^2 which we can write as $(a-ib)(a+ib)=a^2+b^2$. This is correct when a, b are numbers. But when a, b are operators, we have to be careful with the position of the operators since they may not commute. In general, for operators, we perform $(\hat{a}-i\hat{b})(\hat{a}+i\hat{b}) = \hat{a}^2+i\hat{a}\hat{b}-i\hat{b}\hat{a}+\hat{b}^2 = \hat{a}^2+\hat{b}^2+i[\hat{a},\hat{b}]$. Since $\hat{x}, \hat{p}$ do not commute, so, this commutator will appear for us. Let us define

$$\hat{A} = \hat{x}+i\frac{\hat{p}}{m\omega}, \qquad \hat{A}^{\dagger} = \hat{x}-i\frac{\hat{p}}{m\omega} \qquad --- (2)$$

Then we have

$$A^{\dagger}A = \left(\hat{x}-i\frac{\hat{p}}{m\omega}\right)\left(\hat{x}+i\frac{\hat{p}}{m\omega}\right)$$

$$= \hat{x}^2+\frac{p^2}{m^2\omega^2}+\frac{i}{m\omega}\underbrace{[\hat{x},\hat{p}]}_{i\hbar}.$$

$$= \hat{x}^2+\frac{p^2}{m^2\omega^2}-\frac{\hbar}{m\omega}. \qquad -- (3).$$

Substituting eq(3) in eq(1), we obtain the Hamiltonian as

$$\boxed{H = \frac{1}{2}m\omega^2\hat{A}^{\dagger}\hat{A}+\frac{1}{2}\hbar\omega\hat{\mathbb{I}}} \qquad --- (4)$$

The last term is just a constant energy shift to the entire energy eigenvalue spectrum and its just a constant term to the potential energy minimum. Therefore, its not a term to worry about. Then apart from a constant multiplication $\frac{1}{2}m\omega^2$, we have the factorized Hamiltonian that we wanted. We can infact get rid of this ugly constant multiplication by redefining A as

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\,\hat{A} = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} + \frac{i\hat{p}}{m\omega}\right), \quad \hat{a}^{+} = \sqrt{\frac{m\omega}{2\hbar}}\,\hat{A}^{+} = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} - \frac{i\hat{p}}{m\omega}\right) \quad \text{-- (5b).}$$

$$\Rightarrow \quad \hat{x} = \sqrt{\frac{\hbar}{2m\omega}}\left(\hat{a}^{+} + a\right), \quad \hat{p} = i\sqrt{\frac{m\omega\hbar}{2}}\left(a^{+} - a\right) \quad (\text{Hermitian}) \quad \text{-- (5b)}$$

(Recall from previous chapter that $\kappa^{-1} = \sqrt{\frac{\hbar}{m\omega}}$ is a length scale, equal to the distance to the classical turning point which gives the decay length or uncertainty in position of the wavepacket outside the classical turning point.)

These operators a, a^{+} do not commute, and their commutator value is related to the commutator value of $\hat{x}$ and $\hat{p}$. We can obtain that (H.W.)

$$\boxed{[\hat{a}, \hat{a}^{+}] = \frac{1}{i\hbar}[\hat{x}, \hat{p}] = 1} \quad \text{--- (6)}$$

Substitituting eq(5) in the Hamiltonian, we get a simple from

$$\boxed{\hat{H} = \hbar\omega\left(\hat{a}^{+}\hat{a} + \frac{1}{2}\right)} \quad \text{—- (7).}$$

We already have the eigenvalue solutions of the S.H.O from the previous chapter which is $\hbar\omega(n+1/2)$ where 'n' is integer. Therefore, we anticipate that the Hermitian operator $a^{+}a$ has the eigenvalue of 'n'. Indeed, that is going to be the case and we will call $\hat{a}^{+}\hat{a}$ as a counting or number operator. But we dont want to solve this operator $a^{+}a$, because that's same as solving the Hamiltonian itself. Rather we have done all the hard work above to try to exploit the factorized form of the Hamiltonian.

• Ground state :

This is the abstract operator's eigenvalue spectrum we want to solve now. The reason for factorizing the Hamiltonian will now become clear, because thats what we are going to utilize now. Suppose, we consider a general, normalized state $|\psi\rangle$, and look for the expectation value of $\hat{H}$, then we have

$$E = \langle\psi|H|\psi\rangle = \hbar\omega\langle\psi|a^{+}a|\psi\rangle + \frac{1}{2}\hbar\omega\langle\psi|\psi\rangle$$

$$= \hbar\omega\langle a\psi|\underbrace{a\psi}_{\psi'}\rangle + \frac{1}{2}\hbar\omega. \quad -(8)$$

So, we see that the expection value of energy simply becomes an inner product of a new state $|\psi'\rangle = a|\psi\rangle$.

Remember that $\hat{a}$ is not an Hermitian operator, therefore we should not look for the eigenspectrum of this

$\hat{a}$ operator (although we can, and those eigenvectors are complicated, called coherent states that we will learn in QFT course). Rather, we will just study the inner product

$$\langle\psi'|\psi'\rangle = \langle a\psi|a\psi\rangle \geq 0 \quad --- \quad (9)$$

Because, according to one of the axioms of the vector space is that the inner product of all states must be positive definite, and it can only be zero when the state itself is zero. (This makes sense from the physical ground also because the inner product gives us the probability which is always positive).

Now, since this inner product in eq (9) is always positive and ω is also positive, therefore, all energies of the Hamiltonian in eq (8) are positive. We still don't have a justification on why the energies will be quantized though. But we can actually say something about the ground state. A ground state, by definition, is the state that corresponds to the lowest possible energy state. From eq (8), its clear that the lowest possible state is when $\langle a\psi|a\psi\rangle = 0$. From eq (9), this is possible when the state itself is zero. This means

$$\hat{a}|\psi_0\rangle = 0 \quad . \quad \cdots \quad (10)$$

Therefore, the ground state of a S.H.O oscillator is the state $|\psi_0\rangle$ which is being destroyed or annihilated by the operator $\hat{a}$. Note that eq (10) is not an eigenvalue equation of $\hat{a}$ with zero eigenvalue. Although one can think of it because of the fact that $0|\psi\rangle = 0$, but we don't want to call it an eigenvalue equation because $\hat{a}$ is not a Hermitian operator. There are issues with orthogonalization for the eigenstates of a non-Hermitian operator. And we want to built a Hilbert space of the Hamiltonian & $\hat{a}^{+}\hat{a}$ starting with $|\psi_0\rangle$ being its ground state. Rather we will denote $|\psi_0\rangle$ as a ground state given that its destroyed or annihilated by the operator $\hat{a}$. This is why $\hat{a}$ is called destruction/annihilation operator. Then $\hat{a}^{+}$ will be called a creation operator which will take us from the ground state to the excited states as we will see now. In that way, $\hat{a}$ will take us from the excited state back to the ground state. This is why $\hat{a}, \hat{a}^{+}$ are also called ladder operator. The ground state $|\psi_0\rangle$ of such a factorized Hamiltonian is called vacuum state, because its the eigenstate of $\hat{a}^{+}\hat{a}$ with zero eigenvalue. Since $\hat{a}^{+}\hat{a}$ will be called counting or number operator, so, the ground state is something that gives $n=0$, as if it contains no particle. As of now, however, we will refrain from calling it a vacuum state and simple call it the ground state of the S.H.O. The form of $|\Psi_0\rangle$ can be obtained by solving eq(10) in the position basis $|x\rangle$: $\langle x|\Psi_0\rangle = \Psi_0(x)$. Multiplying $\langle x|$ from left we have

$$\langle x|\hat{a}\underset{\uparrow\ \mathbb{I} = \int dx' |x'\rangle\langle x'|}{|}\Psi_0\rangle = 0.$$

$$\int dx' \langle x|\hat{a}|x'\rangle \Psi_0(x') = 0.$$

$$\langle x'|\hat{a}|x\rangle = \sqrt{\frac{m\omega}{2\hbar}}\left[\underbrace{\langle x|\hat{x}|x'\rangle}_{x\,\delta(x-x')} + \frac{i}{m\omega}\underbrace{\langle x|\hat{p}|x'\rangle}_{i\hbar\frac{\partial}{\partial x}\delta(x-x')}\right].$$

So, we have

$$\sqrt{\frac{m\omega}{2\hbar}}\int dx' \left(x - \frac{\hbar}{m\omega}\frac{\partial}{\partial x}\right)\delta(x-x')\,\Psi_0(x') = 0.$$

$$\Rightarrow \boxed{\left(x + \underset{\uparrow\ K^{-2} = \frac{\hbar}{m\omega}}{\frac{\hbar}{m\omega}}\frac{\partial}{\partial x}\right)\Psi_0(x) = 0} \quad --(11).$$

(This is another advantage of using the operator approach that we don't need to solve a 2nd order differential equation. We only have to solve a 1st order differential equation, and as we will see below, we have to solve it only for the ground state and the excited states will be obtained by simply applying the creation operator a^+.)

The solution of eq (11) is very simple:

$$\int d\psi = K^2 \int x\, dx$$

$$\Rightarrow \psi_0(x) = N_0\, e^{-K^2 x^2/2} ,$$

which is a simple Gaussian with the variance K^{-2}, as expected from the solution obtained earlier. We can normalize the Gassian wavepacket to obtain $N_0 = \left(\frac{K}{2\sqrt{\pi}}\right)^{1/2}$. So we write the ground state energy & wavefunction as

$$E_0 = \frac{1}{2}\hbar w \;; \qquad \psi_0(x) = \left(\frac{K}{2\sqrt{\pi}}\right)^{1/2} e^{-K^2 x^2/2} . \quad \text{--} \; \text{⑫}$$

which matches exactly the earlier results.

- **Excited states:** As we promised, we will be able to generate all the excited states from the ground state. For that purpose, we need to work out few identities and commutators first.

Let us define a number or counting operator

$$\hat{N} = \hat{a}^{+} \hat{a} \qquad \text{--} \; (13)$$

This is clearly a Hermitian operator and commutes with the Hamiltonian. Therefore, $\hat{H}$ & $\hat{N}$ share the same eigen-states and the states we are developing are indeed the eigenstates of the number operator $\hat{N}$ with integer eigenvalues.

In the present case, the Hamiltonian linearly depends on the number operator and hence everything is simple. There may arise cases where the Hamiltonian depends on some algebric power of $\hat{N}$, in which case we don't get equally spaced eigenvalues. Nevertheless, choosing the Hilbert space basis of the number operator, which has the unique definition of a factorized form of $a^{+}a$, always helps solving such Hamiltonians easily. It makes things so simple that we will introduce such operators by hand even if the Hamiltonian is not in this form of p^2+x^2. Then every other operators including the Hamiltonian have to be expressed in terms of a^{+} and a. This procedure is called the second quantization procedure.

So, far we know that $|\psi_0\rangle$ is an eigenstate of $\hat{N}$ with zero eigenvalue (recall that $|\psi_0\rangle$ is not an eigenstate of $\hat{a}$ though).

$$\hat{N}\,|\psi_0\rangle = \hat{a}^{+}\hat{a}\,|\psi_0\rangle = 0\,|\psi_0\rangle \quad \text{---}(14)$$

Now if $\hat{a}$ annihilates the ground state $|\psi_0\rangle$, a^{+} cannot annihilate it. In fact, because a, a^{+} do not commute, as we have seen in the discussion of uncertainty principles above, if two operators do not commute, their uncertainties cannot be made arbitrarily zero, rather bounded by the value of the commutator.

So, we have $[a, a^\dagger] = \mathbb{I}$. $\Rightarrow$ $a a^\dagger - \underbrace{a^\dagger a}_{\hat{N}} = \mathbb{I}$.

Acting this commutator on the ground state we get.

$$[a, a^\dagger]|\psi_0\rangle = \mathbb{I}|\psi_0\rangle \Rightarrow a a^\dagger|\psi_0\rangle - \underset{= 0 \text{ from eq (14)}}{\hat{N}|\psi_0\rangle} = |\psi_0\rangle$$

$$\Rightarrow \quad a \underbrace{a^\dagger|\psi_0\rangle}_{|\psi_1\rangle} = |\psi_0\rangle \quad \text{— (15)}$$

(To emphasize again, see how the ordering of operators makes a whole lot of changes. It's so important that there are convention of how to order these creation & annihilation operators).

In what follows, $a^\dagger|\psi_0\rangle$ gives a new state that we denote as $|\psi_1\rangle = a^\dagger|\psi_0\rangle$. We can keep applying $a^\dagger$ again on $|\psi_0\rangle$ to get another state $|\psi_2\rangle$ and so on. Therefore, we can get a hierency of states by simply applying $a^\dagger$ operator again and again:

$$|\psi_n\rangle = \frac{1}{\Omega_n}(a^\dagger)^n|\psi_0\rangle \quad \text{-- (16).}$$

What's it good for? We will see that these states are going to be the eigenstates of $\hat{N}$ operator and hence of the Hamiltonian. This means all these states are linearly independent. So, we need to evaluate

$$\langle\psi_m|\psi_n\rangle = \langle(a^\dagger)^m\psi_0|(a^\dagger)^n\psi_0\rangle\frac{1}{\Omega_n\Omega_m}$$

$$= \langle\psi_0|a^m(a^\dagger)^n|\psi_0\rangle\frac{1}{\Omega_n\Omega_m} \quad \text{--- (17a)}$$

and $\hat{N}|\psi_n\rangle \overset{?}{=} n|\psi_n\rangle$ —— (17b).

- We see that to evaluate these inner product we need to play with a lot of commutators, e.g. $[\hat{N}, \hat{a}]$, $[\hat{N}, \hat{a}^{+}]$ etc. Lets first evaluate them.

$$[\hat{N}, \hat{a}] = [a^{+}a, a] = \underbrace{[a^{+}, a]}_{=-1.} a + a^{+} \underbrace{[a, a]}_{=0.} = -\hat{a}. \qquad -(18a)$$

$$[\hat{N}, \hat{a}^{+}] = \hat{a}^{+}. \qquad -(18b)$$

$$\begin{aligned}[\hat{N}, \hat{a}^{m}] &= [\hat{N}, \hat{a}^{m-1}\hat{a}] = a^{m-1}[N, a] + [\hat{N}, \hat{a}^{m-1}]a \\ &= -a^{m} + [N, a^{m-1}]a = -a^{m} - a^{m} + [N, a^{m-2}]a \\ &= -2a^{m} - a^{m} + [N, a^{m-3}]a \\ &= -m\, a^{m}. \qquad -(18c)\end{aligned}$$

$$[\hat{N}, (\hat{a}^{+})^{m}] = m(a^{+})^{m} \qquad -(18d)$$

$$\begin{aligned}[a, (a^{+})^{m}] &= [a, (a^{+})^{m-1}]a^{+} + (a^{+})^{m-1}[a, a^{+}] \\ &= [a, (a^{+})^{m-2}](a^{+})^{2} + (a^{+})^{m-1} + (a^{+})^{m-1}. \\ &= m(a^{+})^{m-1}. \qquad -(18e)\end{aligned}$$

$$[a^{+}, a^{m}] = -m\, a^{m-1}. \qquad -(18f)$$

- Now we can go back to eq(17b):

$$\hat{N}\,|\psi_n\rangle = \hat{N}\frac{1}{\Omega_n}(a^+)^n\,|\psi_n\rangle = \frac{1}{\Omega_n}\Big(n(a^+)^n + \underbrace{(a^+)^n\,\hat{N}\Big)\,|\psi_0\rangle}_{\hat{N}|\psi_0\rangle = 0|\psi_0\rangle}$$

$$= \frac{1}{\Omega_n}n(a^+)^n\,|\psi_0\rangle$$

$$= n\,|\psi_n\rangle \qquad — \qquad (19).$$

Therefore, $|\psi_n\rangle$ is an eigenstate of $\hat{N}$ with eigenvalue n. Therefore, the nomenclature of $\hat{N}$ being a number or counting operator is justified.

- $$\langle\psi_m|\psi_n\rangle = \langle\psi_0|\,a^m(a^+)^n\,|\psi_0\rangle \qquad \text{from (17a).}$$

$$= \langle\psi_0|\,a^{m-1}\,\underbrace{a(a^+)^n}\,|\psi_0\rangle$$

$$= \langle\psi_0|\,a^{m-1}\{n(a^+)^{n-1} + (a^+)^n a\}\,|\psi_0\rangle \qquad \xrightarrow{} a|\psi_0\rangle = 0.$$

$$= \langle\psi_0|\,n\,a^{m-1}(a^+)^{n-1}\,|\psi_0\rangle$$

$$\left.\begin{aligned} &= \langle\psi_0|\,n(n-1)\cdots(n-m)\,(a^+)^{n-m}\,|\psi_0\rangle \\ &= 0 \end{aligned}\right\} \text{ if } m < n.$$

or
$$\left.\begin{aligned} &= \langle\psi_0|\,n(n-1)\cdots 1\;a^{m-n}\,|\psi_0\rangle \\ &= 0 \end{aligned}\right\} \text{ if } m > n$$

or
$$\left.\begin{aligned} &= \langle\psi_0|\,n(n-1)\cdots 1\,|\psi_0\rangle \\ &= n!\,\underbrace{\langle\psi_0|\psi_0\rangle}_{=1.} \\ &= n! \end{aligned}\right\} \text{ if } m = n.$$

$$= n!\;\delta_{mn}.$$

Therefore, $|\psi_n\rangle = \frac{1}{\sqrt{n!}} (a^+)^n |\psi_0\rangle$. ---(20)

(Some books simply write $\boxed{|n\rangle}$ instead of $|\psi_n\rangle$). These are the eigenstates of the number operator $\hat{N}$, & hence are the eigenstates of the Hamiltonian with the eigenvalues $(n+1/2)\hbar\omega$ as obtained to be :

$$\boxed{\begin{aligned} \hat{H}|\psi_n\rangle &= \hbar\omega(\hat{N}+1/2)\,|\psi_n\rangle \\ &= \hbar\omega(n+1/2)\,|\psi_n\rangle \end{aligned}} \quad ---(21).$$

- a^+, a as Raising and Lowering operators (Ladder op.).

$$\begin{aligned} a^+|\psi_n\rangle &= \frac{1}{\sqrt{n!}}(a^+)^{n+1}|\psi_0\rangle \\ &= \frac{1}{\sqrt{(n+1)!}}\sqrt{n+1}\cdot(a^+)^{n+1}|\psi_0\rangle \end{aligned}$$

$$\Rightarrow \boxed{a^+|\psi_n\rangle = \sqrt{n+1}\,|\psi_{n+1}\rangle} \quad ---(22a)$$

$$\begin{aligned} a|\psi_n\rangle &= \frac{1}{\sqrt{n!}}\,a(a^+)^n|\psi_0\rangle \\ &= \frac{1}{\sqrt{n!}}\big(n(a^+)^{n-1} + \underbrace{(a^+)^n a\big)|\psi_0\rangle}_{=0 \text{ since } a|\psi_0\rangle = 0.} \qquad \text{using eq (18e)} \end{aligned}$$

$$\Rightarrow \boxed{a|\psi_n\rangle = \sqrt{n}\,|\psi_{n-1}\rangle} \quad -(22b).$$

Eqs (22a) and (22b) justify the name that $\hat{a}^{+}$ and $\hat{a}$ are the raising and lowering operator since they take to to one higher and lower states respectively. They both together are also called the ladder operator.

(H.W) using these lowering and raising operator properties of $\hat{a}$, and $\hat{a}^{+}$, prove that $\hat{N}|\psi_n\rangle = n|\psi_n\rangle$ and $[a, a^{+}]|\psi_n\rangle = |\psi_n\rangle$.

- Wave functions of excited states:

→ We have already computed the wave function of the ground state by solving the 1st order differential equation $\langle x|a\psi_0\rangle = 0 \Rightarrow a\psi_0(x) = 0$. which gave us (eq (12))

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2} = \left(\frac{\kappa}{\sqrt{\pi}}\right)^{1/2} e^{-\kappa^2 x^2/2}.$$

→ We can now obtain all the excited states by simply operating the a^{+} operator:

$$\psi_1(x) = \langle x|\psi_1\rangle = \langle x|a^{+} \underset{\uparrow}{\,} \psi_0\rangle$$

$\int dx' \, |x'\rangle\langle x'|$ & $\langle x|x'\rangle = \delta(x-x')$

$$= a^{+}(x)\,\psi_0(x)$$

$$= \sqrt{\frac{m\omega}{2\hbar}}\left(x - i\frac{p}{m\omega}\right)\left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2},$$

$$= \sqrt{\frac{m\omega}{2\hbar}}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\left[x - \frac{i}{m\omega}\left(-i\hbar\frac{d}{dx}\right)\right] e^{-\frac{m\omega}{2\hbar}x^2}.$$

$$= (\;''\;)\left[x - \frac{\hbar}{m\omega}\left(-\frac{m\omega}{2\hbar}\right)\cdot 2x\right] e^{-m\omega/2\hbar\, x^2},$$

$$= \left(\frac{K}{2\sqrt{\pi}}\right)^{1/2} \underbrace{2(Kx)}_{\rightsquigarrow\, H_1(x/\alpha)} e^{-m\omega/2\hbar\, x^2} \quad , \because\; K = \sqrt{\frac{m\omega}{\hbar}}$$

← Hermite polynomial.

$$= \left(\frac{K}{2\sqrt{\pi}}\right)^{1/2} H_1(Kx)\, e^{-K^2x^2/2}$$

→ Similarly, n^{th} excited state can be obtained as

$$\psi_n(x) = \frac{1}{\sqrt{n!}}\left(a^{\dagger}(x)\right)^n |\psi_0\rangle$$

(H.W.) $$= \left(\frac{K}{2^n n! \sqrt{\pi}}\right)^{1/2} H_n(Kx)\, e^{-K^2x^2/2} \qquad \cdots (23)$$

This exactly matches the wavefunction we derived in the previous chapter.

- Lets try to evaluate the expectation values of $\hat{x}$ and $\hat{p}$ operators in this number operator's Hilbert space.

$$\langle \hat{x} \rangle_n = \langle \psi_n | \hat{x} | \psi_n \rangle = \langle \psi_n | \sqrt{\frac{\hbar}{2m\omega}} (a + a^\dagger) | \psi_n \rangle$$

$$= \sqrt{\frac{\hbar}{2m\omega}} \Big[\langle \psi_n | \underbrace{a \psi_n}_{\sqrt{n-1}\, |\psi_{n-1}\rangle} \rangle + \langle \psi_n | \underbrace{a^\dagger \psi_n}_{\sqrt{n}\, |\psi_n\rangle} \rangle \Big]$$

and $\langle \psi_n | \psi_m \rangle = 0$ for $m \neq n$.

$= 0$. as expected from the Gaussian wavepacket with center at $x = 0$.

$$\langle \hat{p} \rangle_n = \langle \psi_n | \hat{p} | \psi_n \rangle = \sqrt{\frac{m\omega\hbar}{2}}\, i \langle \psi_n | (a - a^\dagger) | \psi_n \rangle = 0.$$

$$\langle x^2 \rangle_n = \left(\frac{\hbar}{2m\omega} \right) \langle \psi_n | \underbrace{(a + a^\dagger)(a + a^\dagger)}_{} | \psi_n \rangle.$$

$$\underset{=0}{aa} + \underset{=0}{a^\dagger a^\dagger} + \underset{1 + 2aa^\dagger \,=\, 1 + 2N.}{aa^\dagger + a^\dagger a}$$

$$= \frac{\hbar}{m\omega} \left(n + \frac{1}{2} \right)$$

$$\langle p^2 \rangle_n = i^2 \frac{m\omega\hbar}{2} \langle \psi_n | (a - a^\dagger)(a - a^\dagger) | \psi_n \rangle.$$

$$= m\omega\hbar \left(n + \frac{1}{2} \right) = m E_n$$

κ_{cl}.

Uncertainty in position $\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} = \sqrt{\frac{\hbar}{m\omega} (n + 1/2)} = \kappa^{-1} \sqrt{(n + 1/2)}$

$$\Delta p = \sqrt{\langle p^2 \rangle - \langle p \rangle^2} = \sqrt{m\hbar\omega\, (n + 1/2)}.$$

$$\boxed{\Delta p\, \Delta x = \hbar (n + 1/2)}$$

Thats exactly we found in the previous case that the uncertainty in position of all the eigenstates are determined by the corresponding turning points $x_{cl} \sim \alpha$ and since the wavefunctions are the Gaussian wavepacket whose spread in position and momentum are determined by the inverse of each other such that $\Delta p \Delta x \sim \hbar$. Therefore, each wavefunction has the least possible uncertainty in position and momentum. This is the definition of coherent states.

H.W. Prove the virial theorem for the Harmonic oscillator.

- Higher dimensional Harmonics oscillator:

Lets solve for a three dimensional Harmonic oscillator. The Hamiltonian is

$$H = \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + \frac{p_z^2}{2m} + \frac{1}{2} m\omega^2 (x^2 + y^2 + z^2) \quad \text{-(24)}$$

with the same spring constant along all directions. This makes all three frequencies to be equal to $\omega = \sqrt{k/m}$.

We notice that all three directions are independent to each other and hence we can employ separation of variable method to solve the above Hamiltonian. The wavefunction hence can split into a product state

$$|\psi_{n_x, n_y, n_z}\rangle = |\psi_{n_x}\rangle |\psi_{n_y}\rangle |\psi_{n_z}\rangle \quad \text{--- (25a)}.$$

such that as we take a projection onto the position space $|\vec{r}\rangle = |x\rangle|y\rangle|z\rangle$ we get

$$\psi_{n_x, n_y, n_z}(\vec{r}) = \psi_{n_x}(x)\, \psi_{n_y}(y)\, \psi_{n_z}(z) \quad \text{--- (25b)}$$

We can define three sets of creation and annihilation operators $a_x, a_x^\dagger$; $a_y, a_y^\dagger$ and $a_z, a_z^\dagger$ in the same way. Then its easy to see that the Hamiltonian becomes

$$\begin{aligned} H &= \hbar\omega \left(a_x a_x^\dagger + a_y a_y^\dagger + a_z a_z^\dagger + \frac{3}{2} \right) \quad \text{-- (26)}. \\ &= \hbar\omega \left(\hat{N}_x + \hat{N}_y + \hat{N}_z + 3/2 \right). \end{aligned}$$

- Ground state $|\psi_{000}\rangle$ is such that its annihilated by all three a_x, a_y, a_z : $a_i |\psi_{000}\rangle = 0$.

- Excited states $|\psi_{n_x n_y n_z}\rangle = \frac{1}{\sqrt{n_x! n_y! n_z!}} (a_x^{\dagger})^{n_x} (a_y^{\dagger})^{n_y} (a_z^{\dagger})^{n_z} |\psi_{000}\rangle$

- $H |\psi_{n_x n_y n_z}\rangle = \hbar\omega (n_x + n_y + n_z + 3/2) |\psi_{n_x, n_y, n_z}\rangle$

$\Rightarrow \quad H |\psi_n\rangle = \hbar\omega (n + 3/2) |\psi_n\rangle = E_n \psi_n.$

where we have defined an interger $n = n_x + n_y + n_z$.

n	$n_x \; n_y \; n_z$	$E_n \; (\hbar\omega)$	$\|\psi_n\rangle$	degeneracy.
0 (g.s)	0 0 0	$\frac{3}{2}$	$\|\psi_{000}\rangle$	0
1 1st excited state	0 0 1 0 1 0 0 0 0	$3/2$	$\|\psi_{001}\rangle$ $\|\psi_{010}\rangle$ $\|\psi_{100}\rangle$	3-fold.
2	0 1 1 1 1 0 1 0 1 0 0 2 0 2 0 2 0 2	$5/2$	$\|\psi_{001}\rangle$ $\|\psi_{110}\rangle$ $\|\psi_{101}\rangle$ $\|\psi_{002}\rangle$ $\|\psi_{020}\rangle$ $\|\psi_{200}\rangle$	6-fold degeneracy.

- In general, in a 'd'-dimensional Harmonic oscillator, the n^{th} eigenstate is 'n^d'-fold degenerate.

- (H.W.) (i) Show that $|\Psi_n\rangle = |\Psi_{n_x, n_y, n_z}\rangle$ are orthogonal even when $n = n_x + n_y + n_z$ remains the same.

  (ii) Obtain the matrix representation of the Hamiltonian, number operator, $a^\dagger$ & a operators in the infinite dimensional Hilbert space $|\Psi_n\rangle$.

  (iii) Define an unitary operator $\hat{U} = e^{i\phi\hat{N}}$ where ϕ is some number. Act this unitary operator on some wave function Ψ_n. Show that it gives a new wave function as $\Psi_n e^{in\phi}$, which is same as Ψ_n because we know that wavefunction is gauge invariant. Therefore, the number operator is the generator of the gauge transformation or phase transformation. Therefore, if the theory has gauge symmetry, which is true for the global gauge transformations (ie, a constant phase ϕ), then N is a conserved quantity. The reverse is also true that if the theory is a "grand cannonical" kind of ensemble in which number of particle can be arbitrary, then its phase must be fixed or coherent state.

If you have heard of Bose-Einstein condensation, which says photon, phonon, which are a special type of particles with integer spin and often are the quanta of plane-wave solution (but not restricted to it), then such particles all go to the ground state energy at T=0. This is sort of an example of obtaining a fixed phase condition or sometimes say phase condensation. This course is however way to preliminary to study that