Advanced Quantum Mechanics with Applications

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Lecture – 03
The Mathematical Formalism of Quantum Mechanics, Uncertainty Principle

So, in this discussion we shall talk about different representations in quantum mechanics. And it is almost obvious to you that the physical observables would not depend upon the representation that we are using rather should be independent of the representations. So, the expectation values of operators which denote physical observables should remain same.

However, it is possible to go from one representation to another. In particular we are talking about the coordinate representation or the position representation and the momentum representation and we will see that how they are connected. Or rather what is the form of an operator in momentum representation and coordinate representation? And to begin with let us talk about the x operator.

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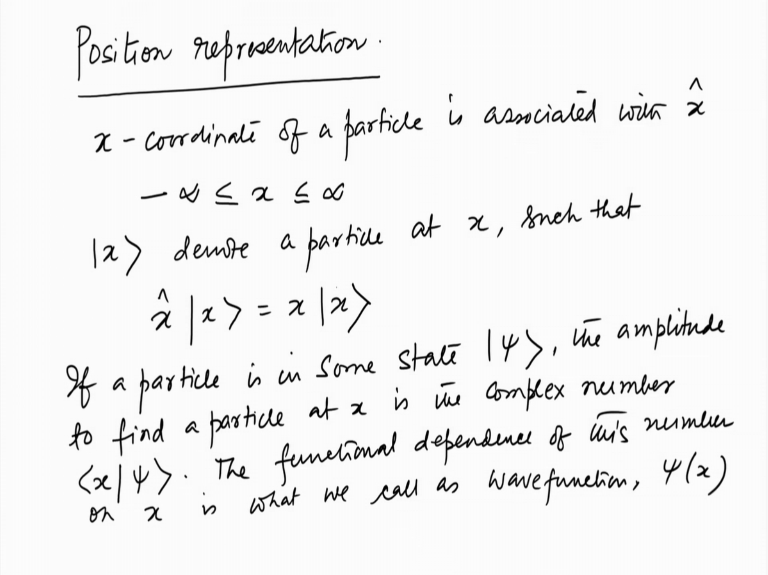

Position representation.

x - coordinate of a particle is associated with $\hat{x}$

$-\infty \leq x \leq \infty$

$|x\rangle$ denote a particle at x, such that

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

If a particle is in some state $|\psi\rangle$, the amplitude to find a particle at x is the complex number $\langle x|\psi\rangle$. The functional dependence of this number on x is what we call as wavefunction, $\psi(x)$

So, we start with position representation. And x coordinate of a particle is associated with the operator x. So, we will write an operator with a hat and so it is associated with x and where of course, my x variable that goes from minus infinity to plus infinity. So, the ket x, so this denote a particle at x such that x cap acting on this ket will give me the position and will return me back the ket and of course, your x cap is a Hermitian operator which will come and for. So, if a particle is in some state psi, psi is an arbitrary state, the amplitude of the particle this is important. The amplitude to find a particle at x is the complex number x psi.

= So basically the functional dependence of this number of this number on x is what we call as wave function psi x. So, let us see so the definition of psi of x is the overlap with x and the arbitrary state psi.

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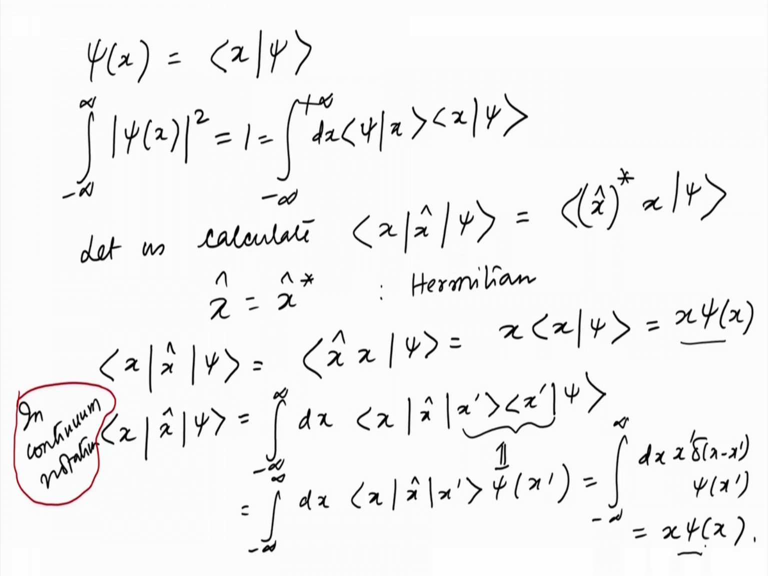

$$\psi(x) = \langle x|\psi\rangle$$

$$\int_{-\infty}^{\infty} |\psi(x)|^2 = 1 = \int_{-\infty}^{+\infty} dx \langle\psi|x\rangle\langle x|\psi\rangle$$

Let us calculate $\langle x|\hat{x}|\psi\rangle = \langle(\hat{x})^* x|\psi\rangle$

$\hat{x} = \hat{x}^*$: Hermitian

$$\langle x|\hat{x}|\psi\rangle = \langle\hat{x}\, x|\psi\rangle = x\langle x|\psi\rangle = \underline{x\psi(x)}$$

In continuum notation

$$\langle x|\hat{x}|\psi\rangle = \int_{-\infty}^{\infty} dx \langle x|\hat{x}\underbrace{|x'\rangle\langle x'|}_{\mathbb{1}}\psi\rangle$$

$$= \int_{-\infty}^{\infty} dx \langle x|\hat{x}|x'\rangle\psi(x') = \int_{-\infty}^{\infty} dx\, x'\delta(x-x')\,\psi(x')$$

$$= x\underline{\psi}(x).$$

So, since the basic postulate says that the total probability of finding the particle should be one between minus infinity to plus infinity. So, we can write this as minus infinity to plus infinity mod psi x square is equal to 1 and that is equal to minus infinity to plus infinity, and you have a dx and then there is a psi x, x psi and so that is the definition.

And now, let us calculate x and x cap psi. So, that tells that this is x cap star and x psi. Now, x is equal to x cap star this is called as the Hermitian operator x has to be a Hermitian operator because x is related to the measurement of the position of the particle. So, it is a physical observable and hence the operators should be Hermitian. So, if this is true then this x cap psi is same as x cap x psi which is same as x x psi and nothing, but x psi x. So, this is the, so x cap operator being taken between these states x which we know that x acting on x cap acting on x will give me x and we will return the ket x and so that is now, taken with this with an arbitrary state psi and it gives me the position of the particle x and returns me the wave function which is the function of x.

So, if you want to do the same calculation in a continuum notation. So, this is in discrete notation where we have extensively used the Dirac bra and ket formalism if you want to do it in. So, let us write it in continuum notation is the same thing excepting that, we are writing it in continuum notation now. So, it is this and this is minus infinity to plus infinity dx and x x cap and x prime and so this is psi. So, we have simply introduced states completeness of states and this is nothing, but minus infinity to infinity dx and x x cap x prime and a psi of x prime and this is nothing, but minus infinity to plus infinity dx x prime delta x minus x prime and a psi of x prime which is nothing by using the property of the delta function its nothing, but x psi x

So, it is the same thing that we have got here and here we have used to different notations in order to arrive at the same result, all right. So, we are dealing with the position representation and let us now, talk about the momentum operator.

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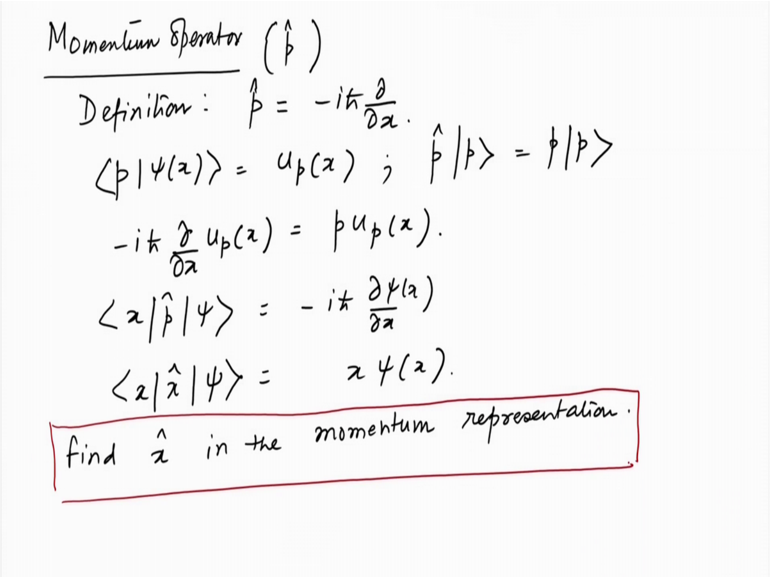

Momentum Operator ($\hat{p}$)

Definition : $\hat{p} = -i\hbar \frac{\partial}{\partial x}$.

$\langle p|\psi(x)\rangle = u_p(x)$; $\hat{p}|p\rangle = p|p\rangle$

$-i\hbar \frac{\partial}{\partial x} u_p(x) = p\, u_p(x)$.

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

$\langle x|\hat{x}|\psi\rangle = x\,\psi(x)$.

find $\hat{x}$ in the momentum representation.

So, the momentum operator is written with a p cap and the definition we can prove this, but however, we will skip the proof and take it as a definition. So, definition is that a p is written as a minus i h cross del del x. So, we may actually define a p and a psi of x to be a state a momentum eigenstate let us call it as u p x, where p this subscript denote the momentum and similarly as earlier. So, it acts on a ket p and returns back the momentum of the particle and the ket itself and so this is nothing, but then minus i h cross del, del x of u p x which is equal to p, u p x.

And similarly when we want to write the expectation of the momentum operator between the position ket x and an arbitrary state psi this is nothing, but minus i h cross del psi del x. And so this if you want to contrast with what we have just obtained in the last slide this is equal to x psi x.

So, as I told you that it is possible to prove the definition of the momentum operator. However, we will skip that rather what we would do is that we will go ahead to prove the form of the position operator in the momentum space. And in order to do that let us the question is find x cap in the momentum representation, ok.

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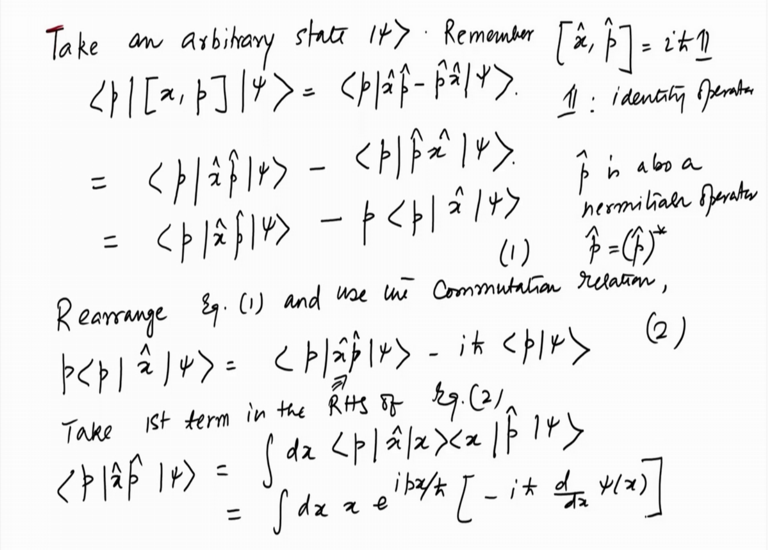

Take an arbitrary state $|\psi\rangle$. Remember $[\hat{x}, \hat{p}] = i\hbar\mathbb{1}$

$$\langle p|[x, p]|\psi\rangle = \langle p|\hat{x}\hat{p} - \hat{p}\hat{x}|\psi\rangle.$$

$\mathbb{1}$: identity operator

$$= \langle p|\hat{x}\hat{p}|\psi\rangle - \langle p|\hat{p}\hat{x}|\psi\rangle.$$

$$= \langle p|\hat{x}\hat{p}|\psi\rangle - p\langle p|\hat{x}|\psi\rangle \quad (1)$$

$\hat{p}$ is also a hermitian operator $\hat{p} = (\hat{p})^*$

Rearrange Eq. (1) and use the commutation relation,

$$p\langle p|\hat{x}|\psi\rangle = \underset{\nearrow}{\langle p|\hat{x}\hat{p}|\psi\rangle} - i\hbar\langle p|\psi\rangle \quad (2)$$

Take 1st term in the RHS of Eq. (2)

$$\langle p|\hat{x}\hat{p}|\psi\rangle = \int dx\, \langle p|\hat{x}|x\rangle\langle x|\hat{p}|\psi\rangle$$

$$= \int dx\, x\, e^{ipx/\hbar}\left[-i\hbar\frac{d}{dx}\psi(x)\right]$$

And to do that let us take an arbitrary. So, an arbitrary state psi and we can use the commutation relation between x and p to be. So, remember x and p the commutation is equal to i h cross, i, where this is an identity operator or you can call it an identity matrix and basically the x and p which are the conjugate variables here they do not commute and the commutation give rise to a finite quantity which is equal to i h cross. And remember that they both are infinite dimensional matrices each of x and p and infinite dimensional matrices do not commute.

So, now, I can write or rather take this commutation relation between the ket p and psi and this is nothing but equal to p x cap, p cap minus, p cap, x cap and a psi. And which is nothing but equal to if I separate it out it is x cap p caps I and minus p p cap x cap psi that is separating it out. Now, we have p x cap p cap, I leave this first term as it is and apply or rather operate p cap on the drop p which gives me a p and so this is equal to a x cap and a psi. So, this is also again taken as momentum is also a Hermitian operator which means a p equal to p star hm

Now, if I write this as equation 1, if I rearrange, equation one and use the commutation relation then I can write this as a p x rather p x psi, equal to a p x p psi and a minus i h cross p psi that is just rearranging this and using the commutation relation and now, take the first term. So, let us call this as to take first term in the right RHS of equation 2 that is this term and this term can be written as a p x cap p caps psi which we use our continuum notation which is equal to p x cap x x again use the completeness of states and this, and this is nothing but this is equal to a dx x exponential i p x by h cross and a minus i h cross d dx of psi x. Now, I leave one step for you to figure out and complete.

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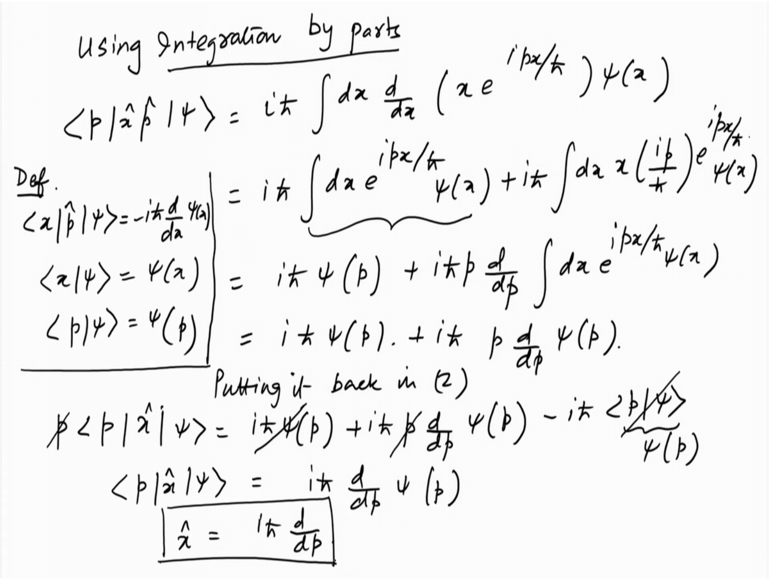

Using Integration by parts

$$\langle p|\hat{x}\hat{p}|\psi\rangle = i\hbar\int dx\,\frac{d}{dx}\left(x\,e^{ipx/\hbar}\right)\psi(x)$$

Def.

$\langle x|\hat{p}|\psi\rangle = -i\hbar\frac{d}{dx}\psi(x)$

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

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

$$= i\hbar\underbrace{\int dx\,e^{ipx/\hbar}\psi(x)} + i\hbar\int dx\,x\left(\frac{ip}{\hbar}\right)e^{ipx/\hbar}\psi(x)$$

$$= i\hbar\psi(p) + i\hbar p\frac{d}{dp}\int dx\,e^{ipx/\hbar}\psi(x)$$

$$= i\hbar\psi(p). + i\hbar\,p\frac{d}{dp}\psi(p).$$

Putting it back in (2)

$$\cancel{p}\langle p|\hat{x}|\psi\rangle = \cancel{i\hbar\psi(p)} + i\hbar\cancel{p}\frac{d}{dp}\psi(p) - i\hbar\underbrace{\cancel{\langle p|\psi\rangle}}_{\psi(p)}$$

$$\langle p|\hat{x}|\psi\rangle = i\hbar\frac{d}{dp}\psi(p)$$

$$\boxed{\hat{x} = i\hbar\frac{d}{dp}}$$

So, using integration by parts, please look at calculus book and or rather mathematical physics book and see what integration by part is and this can be written as. So, this same term I write it here this is equal to a i h cross a dx, and d dx of x exponential i p x by h cross psi x. So, this can be written as i h cross d dx of exponential i p x by h cross psi of x plus i h cross dx x i p over h cross exponential i p x by h cross psi of x. If you do it carefully you will get it.

So, this is nothing, but this is equal to the Fourier transform of psi of x which is nothing, but psi of p. So, this is psi of p and this is i h cross p and a d dp of dx exponential i p x by h cross psi of x. So, this whole thing is written as d dp of this and one can check that that is true its i h cross psi p plus i h cross p d dp of psi of p, ok.

So, this is equal to where of course, we have used definitions such as let us see the definitions being used we have x p psi is equal to minus i h cross d dx of psi of x which is known and x of psi is equal to psi of x and p of psi is equal to psi of p. So, this is our first term on the RHS of 2. If we put it back we will get putting it back in into we will get p. So, we will get up p and p p x sorry p x psi and this is equal to i h cross psi p plus i h cross p d dp of psi p, and minus i h cross p psi and this is nothing but psi p and so there is a plus i h cross psi p and there is a minus i h cross i p they would cancel, and I am going to also lose this p because p is not equal to 0. So, they can be divided by in both sides. And then finally, I land up with a p x cap and a psi which is equal to i h cross d dp of psi p.

So, that is the definition. So, if we want to get the operator x cap in terms of the momentum. So, we will knock off the edge end states and we will get x cap equal to i h cross d dp. So, that is the definition of position operator in the momentum space. As I told you earlier that you are aware of and very familiar with the momentum operator in position space. However, there is an alternate description possible in quantum mechanics where we do not talk about position representation, but we talk about momentum representation, and a position operator takes a form of this kind in the momentum space whereas, the momentum operator in the position space has a minus sign with a del d dx or del del x as you wish to write.

So, this is the position operator of course, this p is in the x direction here is a canonical variable in the x direction corresponding to the x motion. So, let us write down that how would it be.

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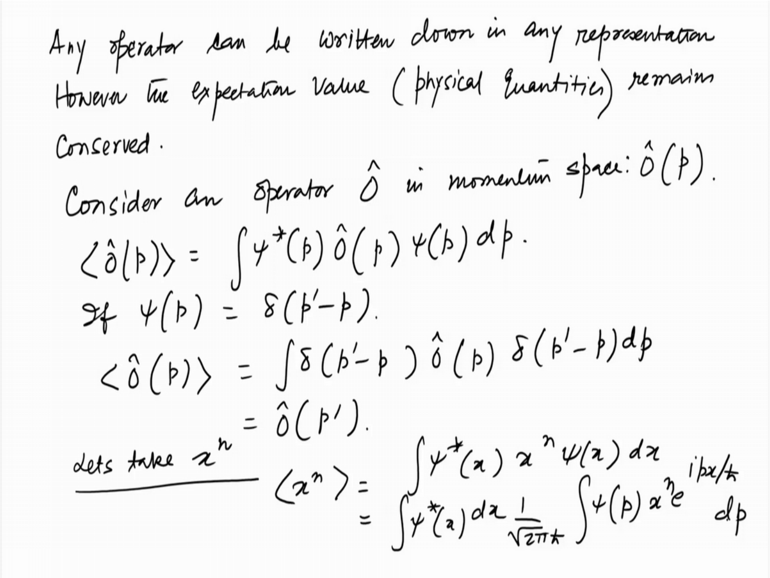

Any operator can be written down in any representation However the expectation value (physical Quantities) remains Conserved.

Consider an operator $\hat{O}$ in momentum space: $\hat{O}(p)$.

$$\langle \hat{O}(p) \rangle = \int \psi^*(p)\, \hat{O}(p)\, \psi(p)\, dp.$$

If $\psi(p) = \delta(p'-p)$.

$$\langle \hat{O}(p) \rangle = \int \delta(p'-p)\, \hat{O}(p)\, \delta(p'-p)\, dp$$

$$= \hat{O}(p').$$

Lets take x^n

$$\langle x^n \rangle = \int \psi^*(x)\, x^n\, \psi(x)\, dx$$

$$= \int \psi^*(x)\, dx \frac{1}{\sqrt{2\pi\hbar}} \int \psi(p)\, x^n e^{ipx/\hbar}\, dp$$

So, any operator can be written down in any representation. However, the expectation value which corresponds to physical quantities remains conserved. Let us write an operator o in momentum space. So, o is written in o p. So, the expectation value of o p is equal to psi star p o p psi p dp psi p if psi of p equal to delta of p prime minus p. Then of course, your o p its equal to a delta p prime minus p, o p delta p prime minus p and dp which gives me nothing, but o p prime.

Sometimes it is important to find powers of the position operator. So, let us take x to the power n. So, x to the power n expectation is written as psi star x x to the power n psi x dx which is equal to psi star x dx and there is a 1 over root over 2 pi h cross and a psi p x to the power n exponential i px by h cross dp. And hence x to the power n or rather, this one exponential i p x by h can be written as minus i h cross d dp whole to the power n exponential i p x by h cross.

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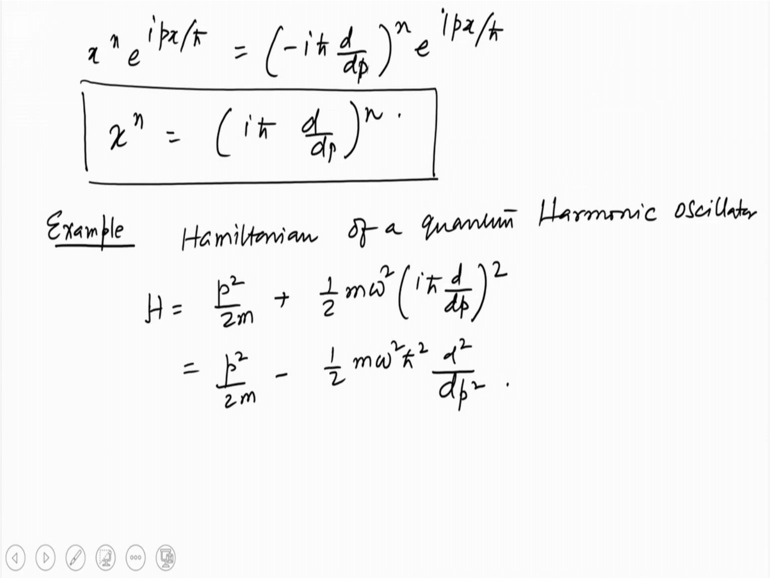

$$x^n e^{ipx/\hbar} = \left(-i\hbar \frac{d}{dp}\right)^n e^{ipx/\hbar}$$

$$\boxed{x^n = \left(i\hbar \frac{d}{dp}\right)^n .}$$

Example Hamiltonian of a quantum Harmonic oscillator

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2\left(i\hbar\frac{d}{dp}\right)^2$$

$$= \frac{p^2}{2m} - \frac{1}{2}m\omega^2\hbar^2\frac{d^2}{dp^2} .$$

See here every time you take a derivative of this exponential function which is oscillatory you would get of x here. So, if you take it n times you will get x to the power n and that is what it is. So, your x to the power n is nothing, but i h cross d d p of n. So, this is the, so if you raise x n times the operator has to be multiplied that many times in order to get it in the momentum space. Let us give a simple example.

So, Hamiltonian of quantum harmonic oscillator: so, this is equal to H equal to p square over 2 m plus half m omega square and then x square. So, I can write x square as i h cross d dp square which is equal to p square over 2 m minus half m omega square h cross square and d 2, dp 2. So, this is the form of the Hamiltonian in the momentum space and we have to solve a potential or rather Schrodinger equation with this Hamiltonian.

We have always you know solved the quantum harmonic oscillator problem writing it in position space that is changing the p to minus i h cross del del x, and then I have gone ahead and solved the Schrodinger equation. However, an alternate thing can also be done in the form of this.

Let us go to another important discussion which is called as density operators and density matrices.

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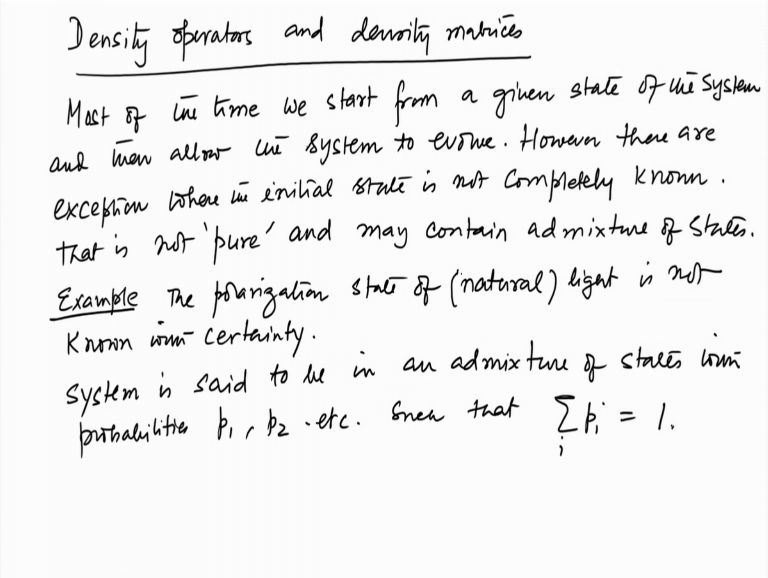

Density operators and density matrices

Most of the time we start from a given state of the system and then allow the system to evolve. However there are exception where the initial state is not completely known. that is not 'pure' and may contain admixture of states.

Example The polarization state of (natural) light is not known with certainty.

System is said to be in an admixture of states with probabilities p_1, p_2 etc. Such that $\sum_i p_i = 1$.

So, the origin of the problem is like this that usually we deal with a large number of particles. When we talk about a particular experiment or even talk about Young's double slit experiment we do not talk about a single photon we talk about a large number of photons. So, there is a statistical analysis or the statistical theory has to be inbuilt.

Now, the statistical probability or the weightage that is associated with the statistical ensemble that has to be taken into account and as well as the probabilistic interpretation of quantum mechanics has to be taken into account. So, the problem as in classical statistical mechanics which was only the probabilistic interpretation or the probability was coming as a weights of the statistical you know the entities is no longer true. We also have a quantum mechanical probabilistic interpretation which comes and interferes with that. So, in order to develop the quantum statistical mechanics it is important to study these density operators or the density matrix and we will give you the important points and probably do one or two examples with that.

Most of the time or ok, I mean which is true as well you can ah say that there are exceptions to this as well. So, most of the time we worry about we start from a given state of the system and then allow the system to evolve. However, there are exceptions where the initial state is not completely known. We will say it in a little technical words, we will say that that is not pure and may contain admixture of states.

So, this is an example can be given as the polarization state of natural light what we mean by is not laser it is basically natural light is not known with precision, with certainty. Which means that there are different polarizations that are mixed for sure we know that the amplitude is actually could be in any direction and this called as a polarization being not in a given direction or its not known. And then in this particular case that system is said to be in an admixture of states, states with probabilities p 1 p 2 etcetera such that sum over i p i is equal to 1.

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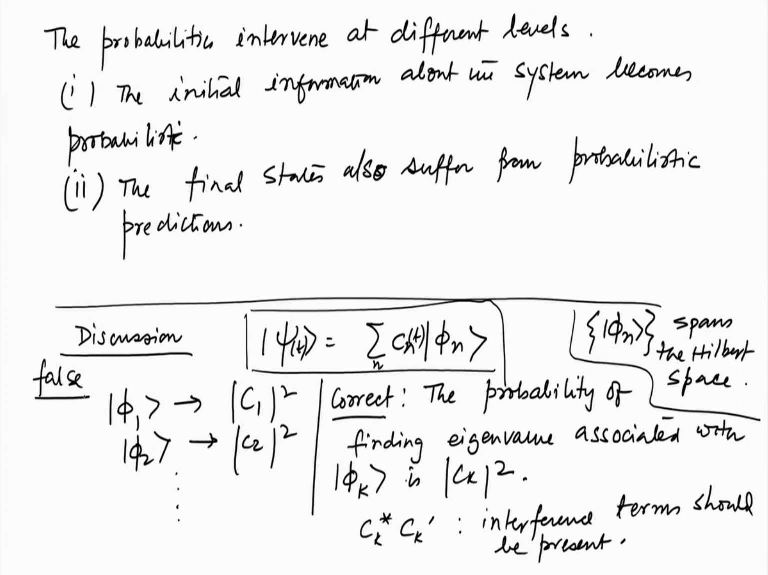

The probabilities intervene at different levels.

(i) The initial information about the system becomes probabilistic.

(ii) The final states also suffer from probabilistic predictions.

Discussion

$$|\psi(t)\rangle = \sum_n c_n(t)|\phi_n\rangle$$

$\{|\phi_n\rangle\}$ spans the Hilbert space.

false

$|\phi_1\rangle \rightarrow |C_1|^2$

$|\phi_2\rangle \rightarrow |C_2|^2$

⋮

Correct: The probability of finding eigenvalue associated with $|\phi_k\rangle$ is $|C_k|^2$.

$C_k^* C_{k'}$: interference terms should be present.

So, what I mean to say is that the probabilities intervene at different levels the initial information about the system ballistic. So, it becomes probabilistic and the final states that is the time evolved states also suffer from probabilistic predictions.

So, we will talk about density operators, but while we talk about these probabilistic interpretation, I it one thing that comes to my mind is that sometimes the students get quite confused with the fact that we write. So, this is just a discussion which is slightly out of the way, but it is important never the less. The discussion is that that we write a total state psi and write it in terms of C n and a phi n, where C ns are they depend on time whereas, the basis states phi n s are constants. So, phi n is a basis that spans the Hilbert space.

So, it is often said that the probability to find the state in phi 1 is associated with C 1 square and phi 2 is associated with C 2 square and so on. But this statement is not correct because the cut the correct statement would be the probability to find the eigen function or rather to find an eigen value corresponding to phi 1. So, the correct statement is the probability of finding eigen value associated with phi k is C k square. Because you have to allow for because if you say that the probability that the state is in is found in phi 1 is C 1 mod square phi 2 is C 2 mod square that defeats the purpose of quantum mechanics because there has to be necessarily interference between these states. So, those interference terms such as a C k star and a C k prime interference terms should be present.

So, just to reiterate this when you write a total wave function as a sum of these amplitudes and the basis states there is a sum over n. So, it is not true. So, this is a false or rather this is untrue that the probability of finding the particle in phi 1 is C 1 mod square and phi 2 C 2 mod square and so on. The rather the correct thing is that the probability of finding the eigen value associated with phi 1 is C 1 square C 1 mod square and C 2 mod square and so on, because then that allows for the these the cross terms or the interference terms to be present which are very important for quantum mechanics.

Anyway, we will come back to this density operators and see that what they or density matrices what they see, no, what they actually mean.

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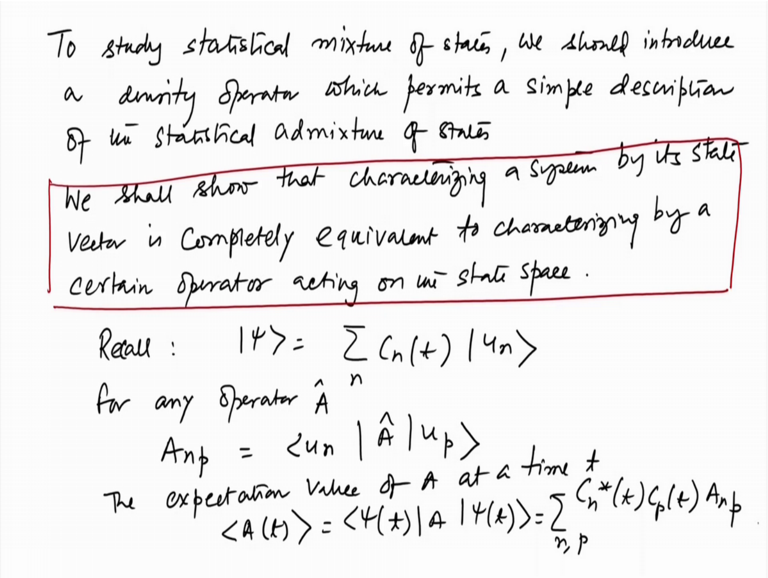

To study statistical mixture of states, we should introduce a density operator which permits a simple description of the statistical admixture of states

We shall show that characterizing a system by its state vector is completely equivalent to characterizing by a certain operator acting on the state space.

Recall : $|\psi\rangle = \sum_n c_n(t)\,|u_n\rangle$

for any operator $\hat{A}$

$$A_{np} = \langle u_n|\hat{A}|u_p\rangle$$

The expectation value of A at a time t

$$\langle A(t)\rangle = \langle\psi(t)|A|\psi(t)\rangle = \sum_{n,p} c_n^*(t)\,c_p(t)\,A_{np}$$

So, to study statistical mixture of states we should use, we should rather introduce a density operator which permits a simple description of the statistical as admixture of states. But also there is another advantage of using the density operator that is without using the state vector or the wave function psi everything could be done in terms of the density operator. So, we shall show that characterizing a system by its state vector is completely equivalent to characterizing it by a certain operator acting on the state space.

So, that underscores the utility of the density operator that we can actually do away with using the state space and completely work with the density operator. So, let me box this rather important statement which we are going to prove.

So, recall that a psi equal to sum over n c n t, u n and for any operator A we can write it O also previously we have written O, but it is a same thing. So, the matrix elements between two basis states u n is given by this. So, the expectation value at a time t is A t, its psi t A psi t this is equal to n and p. So, this is C n t, C p p, A n p, where A n p is defined earlier.

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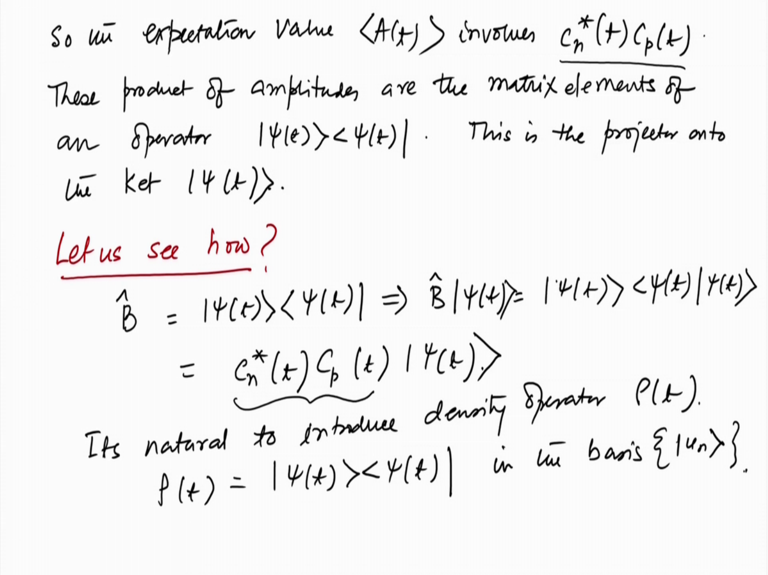

So the expectation value $\langle A(t) \rangle$ involves $\underline{C_n^*(t) C_p(t)}$.

These product of amplitudes are the matrix elements of an operator $|\psi(t)\rangle\langle\psi(t)|$. This is the projector onto the ket $|\psi(t)\rangle$.

Let us see how?

$$\hat{B} = |\psi(t)\rangle\langle\psi(t)| \Rightarrow \hat{B}|\psi(t)\rangle = |\psi(t)\rangle\langle\psi(t)|\psi(t)\rangle$$

$$= \underbrace{C_n^*(t) C_p(t)}_{} |\psi(t)\rangle$$

Its natural to introduce density operator $\rho(t)$.

$\rho(t) = |\psi(t)\rangle\langle\psi(t)|$ in the basis $\{|u_n\rangle\}$.

Now, so the expectation value A t involves these quantities C n star t C p t which are the amplitudes the complex amplitudes. But see that these amplitudes these products of amplitudes are the matrix elements of an operator psi t and psi t. So, so this is this is the projector on to the ket psi t. Let us see how.

So, let us take an operator say let us call this as B which is equal to we will of course, soon change its nomenclature from being B to rho. So, this is equal to a psi of t. So, this tells you the B acting on psi t its equal to a a psi t and a psi p, and psi t, and so on and so this is nothing but a C n star t and C p t and a psi t and so on. So, this is the matrix element or rather the eigen value of this operator. So, this B acting on psi t it will give you this.

So, it is now natural to introduce density operator rho of t, where rho of t is exactly what we said about B that is rho of t is equal to this projector psi t and so on ah. So, in the basis, so psi s are written in the basis this u n, u n's are assumed to be orthonormal basis, but it is not a big problem if they are not there are always going from non orthonormal basis to orthonormal basis by doing a transformation called as a this a Gram-Schmidt Orthogonalization.

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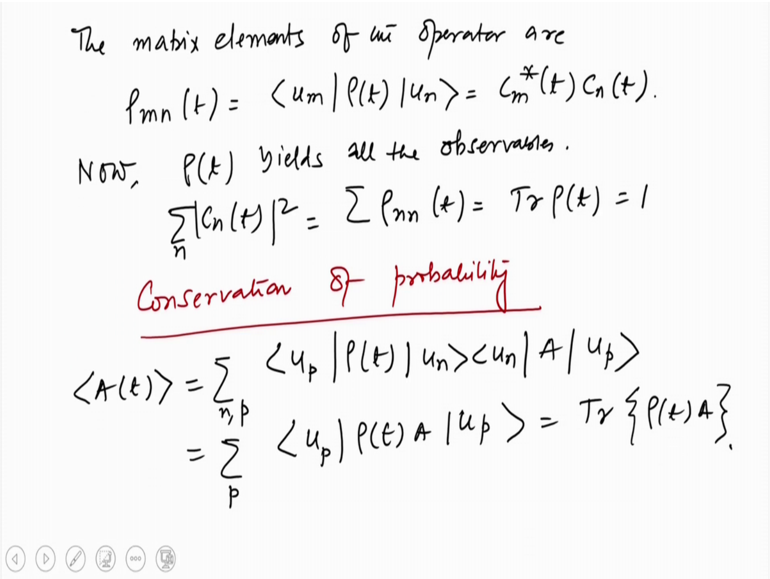

The matrix elements of the operator are

$$\rho_{mn}(t) = \langle u_m|\rho(t)|u_n\rangle = C_m^*(t)\,C_n(t).$$

Now, $\rho(t)$ yields all the observables.

$$\sum_n |C_n(t)|^2 = \sum \rho_{nn}(t) = Tr\,\rho(t) = 1$$

Conservation of probability

$$\langle A(t)\rangle = \sum_{n,p} \langle u_p|\rho(t)|u_n\rangle\langle u_n|A|u_p\rangle$$

$$= \sum_p \langle u_p|\rho(t)A|u_p\rangle = Tr\{\rho(t)A\}.$$

And so this is a, so the matrix elements of the operator are. So, rho mn t equal to u m rho t u m which is equal to cm star t C n t. So, now, rho t yields all the physical observables as was the claim that it will replace the usage of the state vector psi of t. So, before we show that this is so your sum over n C n t mod square it is equal to rho nn t which is equal to trace of rho t which is equal to 1. So, this talks about the conservation of probability.

So, the expectation value of any arbitrary operator is written as u p rho t and a u n, u n A and a u p and this is nothing but summation over p u p, rho t A and u p this and this is nothing but trace of a rho t A. So, we do not; so we simply have to calculate the density matrix multiply it by the operator and take the trace that will give the expectation value of the operator. So, this is completely equivalent.

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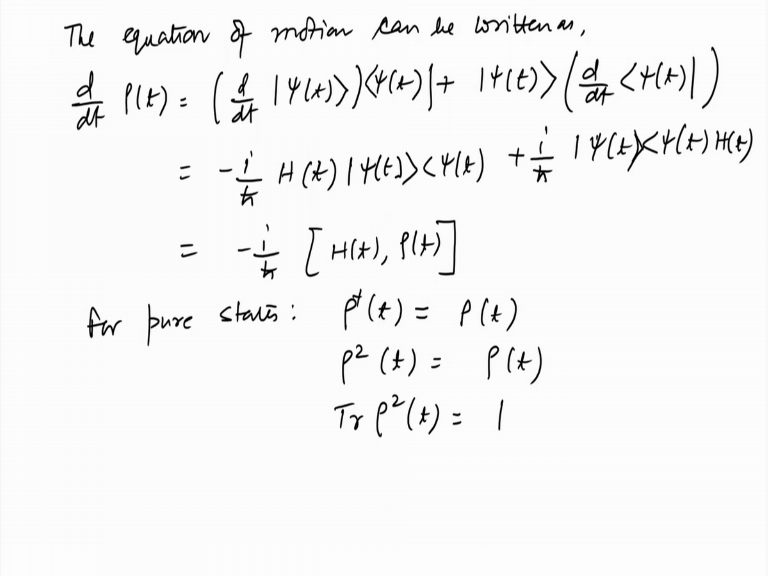

The equation of motion can be written as,

$$\frac{d}{dt}\rho(t) = \left(\frac{d}{dt}|\psi(t)\rangle\right)\langle\psi(t)| + |\psi(t)\rangle\left(\frac{d}{dt}\langle\psi(t)|\right)$$

$$= -\frac{i}{\hbar} H(t)|\psi(t)\rangle\langle\psi(t) + \frac{i}{\hbar}|\psi(t)\rangle\langle\psi(t)H(t)$$

$$= -\frac{i}{\hbar}\left[H(t), \rho(t)\right]$$

for pure states: $\rho^{\dagger}(t) = \rho(t)$

$\rho^{2}(t) = \rho(t)$

$Tr\,\rho^{2}(t) = 1$

And the last thing that we can see is that the equation of motion d dt of rho t its equal to d dt of psi t and psi t outside. Now, keeping that psi t and psi t taking the derivative on the other psi t; so, this is equal to minus i by h cross H t psi t, psi t and this is a plus i by h cross psi t psi t H t, and this is nothing but minus i by h cross H t and rho t. And so this tells that the equation of motion of the density matrix of the density operator is the commutation of the operator with the Hamiltonian. So, if these two commute then they have same state of eigenstates or they have the same basis, they can be diagonalized in the same basis.

So, for pure states, I we have def defined pure earlier it means that the initial state with which we begin with is completely known. So, there is no statistical admixture at all and so for pure states rho dagger of p equal to rho of t, rho square of t equal to rho of t and trace of rho square of t equal to 1. And as I told that if there is an admixture of states some of these properties do not hold good we will see for a particular example.