

Introduction to Statistical Mechanics
Girish S Setlur
Department of Physics
Indian Institute of Technology - Guwahati

Lecture – 25
Introduction to Second Quantisation: Harmonic Oscillator

Okay, so I am going to start a new topic, so this is along the lines of the, so it belongs to the part which I have been calling some of the advanced topics, so in other words if you recall that I had classified some of the topics such as renormalization group, second quantization, Schwinger Dyson equations etc., as advanced topics and so I finished discussing renormalization group applied to the one- D using model.

So, now I am going to discuss the method of second quantization which is very powerful when dealing with interacting many particle systems, so I am going to start with a very simple example which you should all be familiar with but it is worthwhile doing it the way I am going to explain because I am going to use a similar method again and again okay. So, the model I am going to start with is the absolutely simple, one dimensional harmonic oscillator.

(Refer Slide Time: 01:43)

INTRODUCTION TO SECOND QUANTIZATION

$$H = \frac{p^2}{2m} + \frac{1}{2} m \omega^2 x^2 \quad ; \quad [x, p] = i\hbar$$

$$H = E \left(\underbrace{\frac{p^2}{2mE}}_{Y^2} + \underbrace{\frac{m^2 \omega^2}{2E} x^2}_{X^2} \right) \quad ; \quad p = -i\hbar \frac{d}{dx} \quad ; \quad H\psi = E\psi \quad ; \quad E > 0$$

$$X = x \sqrt{\frac{m\omega}{2\hbar}} \quad ; \quad Y = \frac{p}{\sqrt{2m\hbar\omega}}$$

$$[X, Y] = i\hbar \left(\frac{\omega}{2E} \right) = \frac{i\hbar\omega}{2E}$$

$$Y^2 + X^2 = (Y + iX)(Y - iX) + \frac{\hbar\omega}{2E}$$

$$X = \frac{1}{\sqrt{2}} \left(\frac{a + a^\dagger}{\sqrt{2}} \right) \quad ; \quad Y = \frac{1}{\sqrt{2}} \left(\frac{a - a^\dagger}{i\sqrt{2}} \right)$$

$$H = E \left(\frac{a^\dagger a + a a^\dagger}{2} + \frac{1}{2} \right) = E \left(a^\dagger a + \frac{1}{2} \right)$$

So, this is my Hamiltonian so, this is the simple p square by 2m plus 1/2 m omega square x squared, so this is my simple one D Hamiltonian and it is quantum mechanical, so that means the x and p are operators and they obey commutation rules such as this okay, so the question is; the goal is now to find the energy, meaning the eigenvalues of this Hamiltonian.

So, one way is to you know, write the Schrodinger ways to write p as $-i\hbar \frac{d}{dx}$ and then just solve the further stationary states, so this is what one typically does but then you know there is a clever way of doing this, this is actually useful if you also want the Eigen functions along with the Eigen values but if you do not care about the Eigen functions, you only care about the eigenvalues, there is a quicker way of getting it.

And that is through what is called the second quantization method or so basically, it is involves using creation and annihilation operators, so this is; that is going to generalize to something in the context of field, so when I discuss so, this is just a single particle so, in the context of fields we are going to be using a similar method so, I am going to start off with a simpler one particle picture.

So, how do you deal with this; so notice that this has the form so, this resembles something like what I am going to do is the; I am going to first take the liberty of you know multiplying and dividing by a certain energy. So, I am going to multiply okay, so firstly let me do the following. So, I am going to pretend that there is some energy E okay, so which is positive.

And I am going to without loss of generality, multiply and divide by that so, I am going to fix this E later on okay, so I am going to tell you what this E is later on, for now it is just I am at liberty to do this, so long as E is not 0, I have also declared it to be positive so, so long as it is not 0 and it is positive I can always do this because E will cancel out. So, now if you stare at the thing in the bracket, you see this has the form, so it this resembles something like a capital Y squared and this resembles something like capital X squared, okay.

So, these are 2 new operators that I am going to now define, so I am going to define X as the operator X times as square root of $m\omega^2$ divided by $2E$ and the operator Y ; I am going to define as p times 1 over square root of $2mE$. So, now you see the question is; if I look I mean, if Y and X are numbers then, clearly I can always write like this, is not it?

So, I can always write $Y - ix$, so if Y and X are numbers but if Y and X are not numbers, so in general what would this be? Suppose, if I expand this out what will it look like so, this is looks like Y squared right, Y into Y is Y square and if I multiply the ix with $-ix$, it is going to look like x squared but then there is a cross term which is i into XY minus i into YX .

So, notice that if X and Y are numbers or they are just they are not operators, they are just commuting numbers, then X times Y is same as Y times X and this cancels out but then in this example X and Y are operators, so this is actually going to be Y squared plus X squared capital X squared that is, plus i times commutator of capital X capital Y . So, now what is the commutator of capital X , capital Y ?

Just from this; from the definition this is going to look like so, small x commutator, small p is $i\hbar$, so it is going to be $i\hbar$ times the rest of it okay, so the rest of it is basically raised to $1/2$ times ω squared over $4E$ squared okay, so m cancels out and 2 becomes 2 times 2 is 4 and E times E is E square and so, this is going to be $i\hbar$ into ω over $2E$, okay, so that is what that is going to be.

So, this is going to be Y squared plus X squared plus a constant, so that constant happens to be minus $\hbar \omega$ over $2E$, okay. So, now I can do the other way also, so in other words I can choose to do it this way, so notice that these 2 ; if X and Y were numbers it would not matter whether I write it like this or I write it like this, it is the same thing. So but then, so these 2 are not equal in other words, this is not equal to this.

So, what I have to do is I have to write this as this so, I could do this also; I get the different sign here, so I would not do this but I am just pointing out that you could do it this way or this way but I choose to do it this way. So, now Y squared plus X squared is not equal to Y plus iX into Y minus iX but rather it is Y plus iX into; so I have to get rid of this.

So, basically I have to write $\hbar \omega$ plus $2E$, so now it is correct okay, so now it is correct okay, so now it is this is correct okay. So, this is what I am going to use now, okay.

(Refer Slide Time: 08:34)

The image shows a handwritten derivation of the harmonic oscillator Hamiltonian. At the top, the Hamiltonian is written as $H = E \underbrace{(Y+iX)}_{a^\dagger} \underbrace{(Y-iX)}_a + \frac{1}{2}\hbar\omega$. Below this, the ladder operators are defined: $a = Y-iX$ and $a^\dagger = Y+iX$. A bracketed set of equations shows the commutator $[a, a^\dagger] = 2i[X, Y] = \frac{\hbar\omega}{E}$. A note says "choose $E = \hbar\omega$ ". This leads to the commutator $[a, a^\dagger] = 1$. The Hamiltonian is then rewritten as $H = \hbar\omega a^\dagger a + \frac{1}{2}\hbar\omega$, with the energy levels given as $E_n = \hbar\omega(n + \frac{1}{2})$. On the right side, boundary conditions are listed: $a|\psi_0\rangle = 0$ and $H|\psi_0\rangle = \frac{1}{2}\hbar\omega|\psi_0\rangle$. The background of the handwriting includes a phase diagram with labels like "supercritical fluid", "critical point", "triple point", and "gaseous phase".

So, H is going to now look like E times; it is going to look like Y plus iX into Y minus iX times E times this, so it is going to be plus $1/2 \hbar \omega$ okay, so that is what that looks like. So, now what I am going to do is I am going to call this 'a dagger' and I am going to call this 'a' okay. So, a is basically this operator which is equal to Y minus iX and 'a dagger' is going to be Y plus iX okay.

So, dagger means basically, the complex conjugate of the transpose, so it is an operator, so it is the same dagger that you see in quantum mechanics, is the hermitian conjugate. So, now I can ask myself what is this commutator? Notice that this commutator will depend on E because that E was something that I just put in by hand, so I am at liberty to choose E in some convenient way, so to my convenience.

So, notice that this X commutator Y is $i\hbar\omega$ over $2E$, so a commutator, a dagger is basically going to be minus iX commutator Y , then it is going to be Y commutator iX , so there is going to be minus $2i$ there, so this is the answer okay, a commutator a dagger is minus $2i$ times X commutator Y . So, what is X commutator Y ? It is $i\hbar\omega$ over $2E$, so it is the; so this 2 will cancel, i will cancel with minus i and you will get $\hbar\omega$ over E .

So, what I am going to do is; I am going to choose E to be equal to $\hbar\omega$, so if I choose E to be $\hbar\omega$, what is going to happen is that this a , a dagger commutator will be 1 and that will fix the rest of it okay. So, then I will be able to write this Hamiltonian in this fashion, I will be able to write E as $\hbar\omega$ because I have selected it that way, so and this is a dagger a plus $1/2 \hbar \omega$ okay.

So, now you can make out from here that this quantity is a self adjoint positive definite operator, so that means it is a hermitian operator that whose eigenvalues are positive or 0, so you can easily make out what the ground state of the system is because this is either positive or 0, clearly the smallest energy is for a state, so you can select a state where this is 0.

So, if you select a state where which is annihilated by a , so this operator if it annihilates the state, then that is going to be the ground state of the system because that is going to have the lowest energy, so that directly you can make out that has the lowest energy, okay. So, now the question is what about the other Eigen value? So, the ground state is $\frac{1}{2} \hbar \omega$, so how do you make out the other Eigen values?

(Refer Slide Time: 12:16)

$$\begin{aligned}
 |\psi_1\rangle &= a^\dagger |\psi_0\rangle & a a^\dagger - a^\dagger a &= 1 \\
 \langle \psi_1 | \psi_1 \rangle &= \langle \psi_0 | a a^\dagger | \psi_0 \rangle & a a^\dagger &= 1 + a^\dagger a \\
 &= \langle \psi_0 | (1 + a^\dagger a) | \psi_0 \rangle \\
 &= \langle \psi_0 | \psi_0 \rangle + \underbrace{\langle \psi_0 | a^\dagger a | \psi_0 \rangle}_{=0} \\
 &= \langle \psi_0 | \psi_0 \rangle = 1 \\
 |\psi_n\rangle &= \frac{(a^\dagger)^n}{\sqrt{n!}} |\psi_0\rangle & H |\psi_1\rangle &= \hbar \omega a^\dagger a |\psi_1\rangle + \frac{1}{2} \hbar \omega |\psi_1\rangle \\
 & & &= \hbar \omega a^\dagger a^\dagger a |\psi_0\rangle + \frac{1}{2} \hbar \omega |\psi_1\rangle \\
 & & &= \hbar \omega |\psi_1\rangle + \frac{1}{2} \hbar \omega |\psi_1\rangle = \frac{3}{2} \hbar \omega |\psi_1\rangle
 \end{aligned}$$

So, from the ground state you can construct the other states in the following way, so you can construct an excited state, so I am going to call ψ_1 , suppose I define ψ_1 as $a^\dagger \psi_0$, okay so, this is my definition. Now, you can see that this is if ψ_0 is properly normalized, I have to make sure this ψ_1 is normalized. So, if I take the adjoint and I take the norm like this, I get $a^\dagger a \psi_0$.

But then $a^\dagger a$ is; so remember $a^\dagger a - a a^\dagger = 1$, so this is going to be $a^\dagger a = 1 + a a^\dagger$ okay, so this is going to be $\langle \psi_0 | \psi_0 \rangle + \langle \psi_0 | a a^\dagger | \psi_0 \rangle$. Now, notice that this is 0, okay so, this is going to be $\langle \psi_0 | \psi_0 \rangle$ which is 1, so this is properly normalized state. So, now I have to make out, I have to find out what is the energy of the state.

So, the energy of this state will be obtained, first I want to know whether this is the Eigen state or not so, if I take $H \psi_1$, I will get $\hbar \omega$ into a dagger a into ψ_1 plus $1/2 \hbar \omega$ into ψ_1 . So, now this is $\hbar \omega$ into a dagger a into a dagger ψ_0 plus $1/2 \hbar \omega$ into ψ_1 . So, now what is this again; I can rewrite this as; a , a dagger is 1 plus a dagger a .

So, now a dagger a acting on ψ_0 is 0, so this is one contribute, so what will contribute will be 1, so it is $\hbar \omega$ a dagger acting on, so this is effectively 1, so this a dagger behaves like 1 against acting on ψ_0 , so then a dagger acting on ψ_0 is against ψ_1 and this is $1/2 \hbar \omega$ ψ_1 which is $3/2 \hbar \omega$ ψ_1 . So, like that you can generate all the states, so the n th state is going to be a dagger raised to n times ψ_0 .

But then you will have to normalize this, this will be up to a constant, so you can convince yourself that the correct normalization is this okay. So, notice that the; this is an abstract notation but you can also if you want the Schrodinger picture, you can express Y in terms of P and P as minus $i\hbar d/dx$ and you can go ahead and solve for this differential equations.

So, you see X is going to become $m \omega$ over $2\hbar$ into small x and capital Y is going to become P into 1 over square root of $2m \hbar \omega$ okay. So, how would you write a ? So, a is going to be this operator, so the operator a , that I am talking about so, let me write that operator a as; so a as Y minus iX .

(Refer Slide Time: 15:50)

The image shows handwritten mathematical derivations on a background of a phase diagram. The derivations are as follows:

$$a = Y - iX = \frac{P}{\sqrt{2m\hbar\omega}} - i\sqrt{\frac{m\omega}{2\hbar}} x$$

$$a \psi_0(x) = 0 = \left(\frac{1}{\sqrt{2m\hbar\omega}} - i\sqrt{\frac{m\omega}{2\hbar}} x \right) \psi_0(x) = 0$$

$$= \left(\frac{-i\hbar}{\sqrt{2m\hbar\omega}} \frac{d}{dx} - i\sqrt{\frac{m\omega}{2\hbar}} x \right) \psi_0(x) = 0$$

$$\psi_0(x) = A e^{-\frac{1}{2} x^2}$$

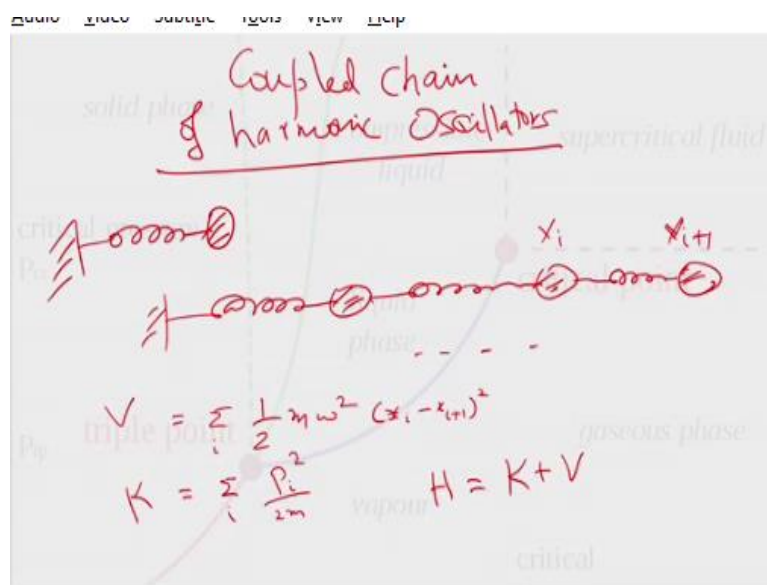
So, a is Y minus iX and so what is Y ; Y is P over square root of $2m \hbar \omega$, so it is $a P$ over square root of $2m \hbar \omega$ and minus i and small x was square root of $m \omega$ over $2\hbar X$, the square root of $m \omega$ over $2\hbar$ times X . So, now the ground state is basically, the one which makes this 0, so now you can think of this as P times square root of $2m \omega$ over $2\hbar X$ acting on ψ_0 to be 0.

Now, what is P ? P is nothing but minus $i\hbar \frac{d}{dx}$ over; okay, so now you can go ahead and solve this and you will be able to write down what is ψ_0 , so ψ_0 will be the solution to this equation which will be some constant into minus e raised to some other constant into x squared, okay, so you can figure out what that is by assuming it is this, at least you can find the λ , this is the normalization which you cannot find.

But substitute that and you will be able to find λ okay, so this is basically how you go about finding the answer to the ground state and the eigenvalues, so the Eigen value of this so that was the ground state Eigen function, so the eigenvalues of this n th state will be; it is going to be this is going to be an integer, so the eigenvalue will be $\hbar \omega$ into n plus $1/2$ because a is an integer, okay so, it is as simple as that.

So, this is how you do creation and annihilation operator approach to a harmonic oscillator okay. So, in the next topic I will try to generalize this and imagine a sequence of coupled one D harmonic oscillators, so that will be the next topic.

(Refer Slide Time: 18:38)



That is coupled chain of harmonic oscillators, so what I have in mind there is so, in the earlier example it was something like this, a mass tied to a spring okay, so that was a 1D harmonic oscillator but now what I have in mind is something like this, you have a mass tied to a spring which is again tied to another mass which is again tied to a spring, which is again tied to a mass and so on and so forth.

So, this is the situation that I have in mind and so I am going to imagine that this is the X_i position of the i th mass and this will be the position of X_{i+1} , so I am going to assume that X_i is the you know is in some sense the deviation from equilibrium okay, so deviation from the unstretched value of the spring. So, as a result you see the potential energy is going to be something like $\frac{1}{2} m \omega^2$, so if all the springs are the same, so it is going to something look like this X_i, X_{i+1} sorry, so the difference between these.

So, it is going to be the difference between these 2, so the distance square, so that is the that is how much potential energy is stored and you sum over all these, so this is the potential energy that is stored, the kinetic energy that is stored is clearly $\sum_i p_i^2 / 2m$. So, now the goal is to see if I can find the eigenvalues of the kinetic plus potential energy of this problem but using the creation and annihilation operator method, Thank you.