Introduction To Statistical Mechanics
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Lecture - 20
Tutorial - II

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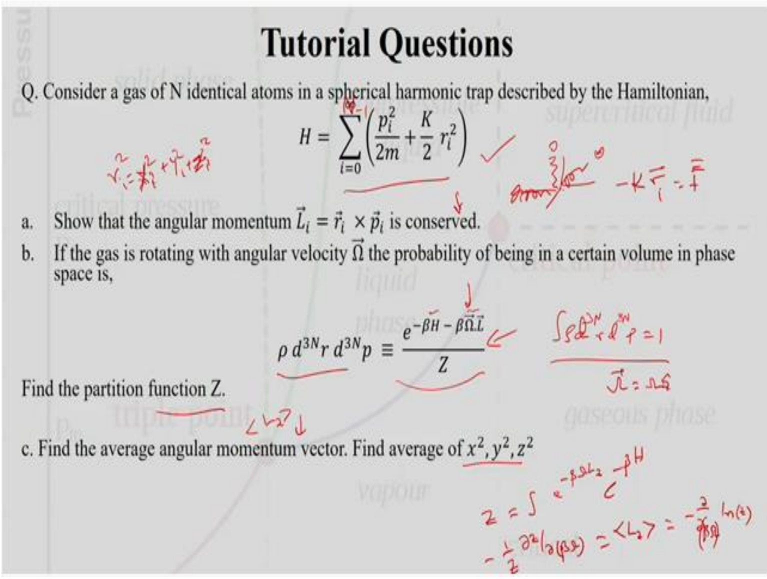

All right, so again I am going to continue with my tutorial questions. So if you remember that in the last tutorial we discussed mainly how to calculate entropy for using combinatorial ideas and specifically we discussed this interesting problem of finding the entropy of a set of charges that are stuck to the corners of a cube. So but now we change tracks a bit and I am going to now start discussing this more physically realistic systems.

So those discrete combinatorial examples are just toy models and they are useful for you know driving home the concept of an of what entropy is? But it really does not help you understand the real world because the real world is not made of you know very simplistic finite systems like that. So specifically in this tutorial I am going to take an example which is quite realistic and that is of a classical ideal gas.

So ideal in the sense that it does not interact with the molecules do not interact with each other but they interact with externally applied fields. So specifically I am thinking of what is known as a harmonic trap. So in other words so think of you know just intuitively you can think of each item to be you know connected by some kind of an imaginary spring to the origin. So each atom is connected to a spring which prevents it from so it can kind of go round and round like this.

I mean it can do anything it wants but there is a cost to running away from the origin so and that cost is basically given by Hooke's law and so you see that it is basically this is the force. So if r_i is the distance from the origin there is a restoring force which is proportional to r_i and in the direction of that so that is effectively what this model is? But you might be wondering why is this realistic because it involves you know connecting subatomic particles to springs.

But then the spring is really a metaphor it is a figure of speech for a potential that goes through a minimum. So in other words you know that any function that has a minimum can be Taylor series expanded around the minimum and the leading term so there is a leading term is the constant and the next leading term is going to be proportional to x^2.

Where x is the so f(x) if it goes from minimum at x = 0, you can always write it as f(0) plus something positive times x^2 and that positive you can identify with ½ k where k is the effective spring constant. So any potential that goes through a minimum can be thought of as due to a spring. So I mean that so in other words the it is just an analogy and so the spring is a metaphor for potential that goes through a minimum.

And practically these harmonic traps nowadays are quite commonly achieved in the context of cold atoms where these traps are typically the criss-crossed laser beams that so the region where the laser beams criss-cross is the place where the atoms you know get trapped through in this harmonic potential. So this is the Hamiltonian of such a system so if you have N atoms and so okay this is up to N only.

So you have okay N - 1. So you have N atoms and so the point is that so there is a kinetic energy and then ri. So $r_i^2 = x_i^2 + y_i^2 + z_i^2$ okay. So the idea is to answer all these questions that follow. So the first question says that show that the angular momentum vector is a conserved quantity okay.
So I have to show that there is a conserved quantity then if the gas is rotating with some angular velocity so I have to show that the probability of being in a certain volume in the phase space is can be thought of as this. So when it is if it is not rotating this is absent. So it is

just $e^{-\beta H}$ /Z so that is the canonical partition function. So when it is rotating with an angular velocity Ω so there is going to be an additional energy associated with the rotation.

So you just think of your classical mechanics where you have this you know the description of dynamical systems in a non-inertial reference frame so that is where this comes from. So basically the energy is going to be the angular momentum times the angular velocity of the non-inertial reference frame. So the idea is to find the partition function by imposing the condition that the total volume in phase spaces is conserved and it is normalized to 1 alright.

So the third question is find the average of the so if Ω is in the z direction. So the idea is to find the average of the angular momentum vector in the z direction and then also the goal is to find the average of the squares of the coordinates themselves. So these are the questions that we want to answer and let us get to it okay. So let us first try and answer the first question and which is this and that is show that the angular momentum is conserved that is fairly obvious.

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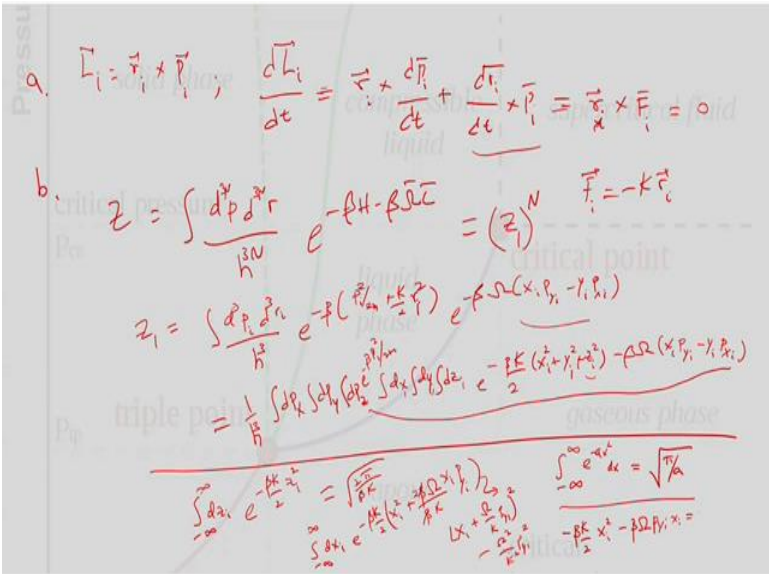

But I am going to do it. So $L_i = r_i \times p_i$. So notice that is a classical mechanics problem so regardless we can always even if it is quantum mechanics it is still true. So I can write this as $r_i \times dp_i/dt + dr_i/dt \times p_i$. So this is velocity and velocity is parallel to momentum because there is no magnetic field and all that. So at that level there is nothing there. So this is 0 and this is nothing but the force.

So that is force applied. So remember I told you the force is given by Hooke's law which is basically a restoring force where the force is proportional to the distance vector and in the negative direction. So this is therefore zero because it is a central force. So as a result the angular momentum of the particles is conserved well in the absence of rotation for this Hamiltonian that is.

So the idea is that if it is rotating you can move to the non-inertial reference frame and then you will pick up a certain rotational energy which is in excess of this Hamiltonian given by Ω.L which gets added on to the Hamiltonian and this is going to be your phase space. This is the probability of finding a particle well it is the probability of finding a i th particle in a volume d^3r_i and d^3p_i in the phase space.

So you know what phase space is it is just a collection of 3 coordinates spatial coordinates and 3 components of the momentum and there are N such particles. So it is basically a 3N dimensional well it is actually 6N dimensional because you know x and p are also there. So there is 2 times 3 times N. So which is a 6N dimensional phase space. So we successfully solved the first part which is very easy it is fairly obvious, it is to show that the angular momentum of each particle is conserved if it is a Hamiltonian of this type.

And this is pretty evident self-evident because it is a central force okay. So part b says if this is your probability distribution in phase space find the partition function. So we are going to use this idea that the total probability is conserved and then what we are called upon to do is called upon to evaluate this integral which is so we have to calculate this basically this is what that is. So this is going to be clearly the answer for 1 particle raise to N okay.

Because that is how it is going to be because they all decoupled. So the particles do not talk to each other they just interact with external fields and the Ω is uniform. So that means Ω is the same for all the particles. So it is just the partition function for 1 particle raise to N at r. So the question is how do you calculate the partition function for one of the particles and that is going to be $Z_1 = \int \frac{d^3p_i d^3r_i}{h^3} e^{-\beta(\frac{p_i^2}{2m}+\frac{k}{2}r_i^2)} e^{-\beta\Omega(x_i p_{y_i} - y_i p_{x_i})}$

So now I am called upon to evaluate this integral so it is ri squared okay. So the question is how do you do this? So the way you do this of course is to make use of the fact that so you might be thinking that well let us try spherical coordinates because there is ri there but then the spherical symmetry is spoiled by this term.

So it is not a good idea. So what we should do is basically write $r_i^2 = x_i^2 + y_i^2 + z_i^2$ and then just use cartesian coordinates. So I am going to do it that way and you see so this is going to be dp_x dp_y dp_z. So I am just writing it out fully. So I really want to take this opportunity to you know display all the steps. So that those of you who are inexperienced in doing these calculations will benefit, those of you already have an idea about how to proceed will probably feel impatient.

So you should just feel free to fast forward and do it on your own or just close this and do it on your own just take it up as a challenge and do it on your own okay. So how does this work? So it is going to look like this. So it is β k/2 x_i^2 + -β Ω(xi pyi – yi pxi). So this is I mean I am going to have to evaluate this integration. So I am going to do this first and then remember that there is a $e^{-\beta(\frac{p_i^2}{2m})}$ outside which I have to do later.

So now let me try and do this. So it is very easy to so remember that if when I try to do this Z it is easy because there is no Z anywhere else. So the Z integration is going to be easy okay. So what is the Z integration z_i. So remember that the components can be positive or negative and there is no restriction and remember this is classical mechanics so momentum and position there is phase space has meaning right.

So I have integrated over position and momenta. So that means the particle can have a well-defined position and momentum at the same time. So all we have to do is calculate this result for so that we will be done with one of the integrations and so remember the standard formula that if you have e raise to -ax squared dx this is nothing but square root of pi/a okay. So yeah so this is square root of pi/a okay. So that is what that is.

So well you can either look this up or this is very standard integration. So I am going to write this as square root of $\sqrt{\frac{2\pi}{\beta k}}$. So this is the answer for that. So now I have to do the other thing. So that means I have to do the x integration the x integration is slightly more complicated because there is a quadratic term there is also a linear term. So there is a standard way of handling this and that is called completing the square.

So for example suppose I want to do the x integration what I am being called upon to do is this integral okay. So this is the integration so I am being called upon to do this. So the way I am going to do this is I am going to do what is called completing the square. So I am going to rewrite - $\beta \frac{k}{2} x_i^2 - \beta\Omega p_{y_i} x_i$. So I am going to rewrite this as so I am going to take this common factor okay let me do that right here.

So I am going to put a bracket here well then I will have to divide by β k. So the β cancels out that is what that is okay. So now this quantity just in the bracket is nothing but

$$(x_i + \frac{\Omega}{k} p_{y_i})^2 - \frac{\Omega^2}{k^2} p_{y_i}^2$$

So there is a cross term. So there is a x squared and there is a cross term which is this. Then there is the term which is quadratic in py which is not present here so I have to subtract it out. So that is what that is so that is called completing the square.

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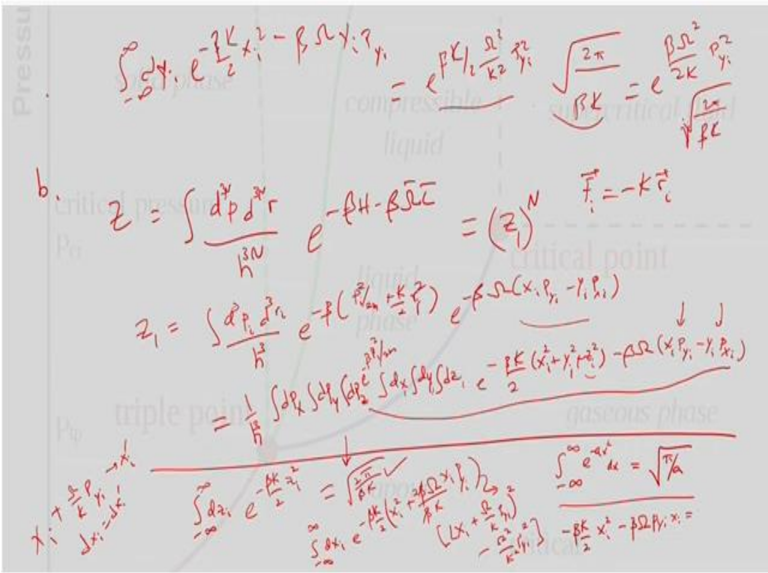

So in other words the integration over the x part is going to be simple because now it is simple because earlier it was this. So now after completing the square it is going to so it is going to be that times the integration over the term which is simple quadratic. So this x_i is just shifted by the constant so as far as the integration over x is concerned p_{yi} is a constant. So I might as well call $x_i + \frac{\Omega}{k} p_{y_i} \rightarrow x'_i$ and then I integrate over.

So dx_i is same as dx'_i and then I integrate over dx_i and I end up getting this result which is $\sqrt{\frac{2\pi}{\beta k}}$ okay. So this is what I get when I complete the square and same thing when I do the y integration. So now I am done with the x, y and z integrations. So I am going to collect all this together and let me display that after collecting them all together okay. So let us go to the next slide okay.

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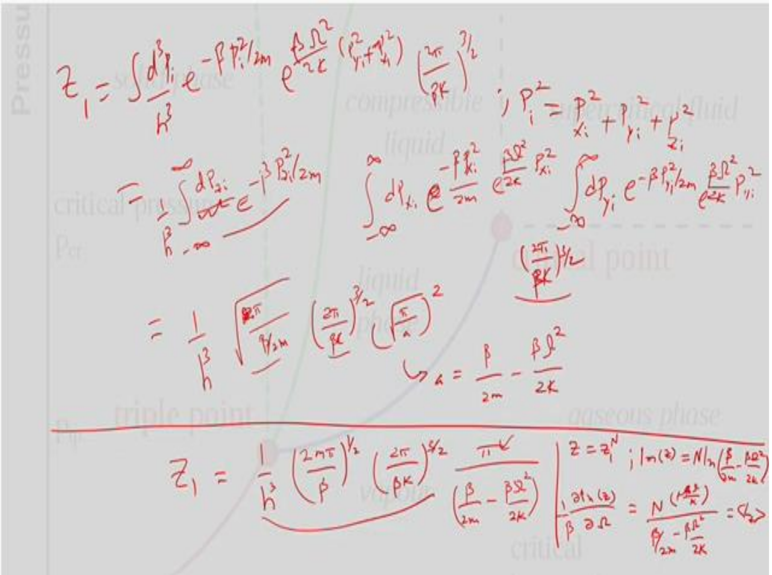

So this the p integration still remains okay whether x integration is done and so the x integration is done and what was the answer. I just have to collect them all together so remember that I did the so when I do the z integration I get this, when I do the x integration I get this then it stands to reason that because x and y are similar because remember there is a inhomogeneous term or the linear term in x and there is a linear term in y as well due to the non-inertial reference frame.

But there is no such term for the z. So for the z the answer is very simple it is this. But for the x and y it is going to be similar to this. So it is for the x integration we got a yi squared for the y integration we are going to get a pxi squared okay. So I am going to use that. So this is going to look like $e^{\frac{\beta\Omega^2}{2k}p_{y_i}^2}\sqrt{\frac{2\pi}{\beta k}}$ okay. So I am going to collect that here.

So it is β Ω squared + pxi squared okay. So that is going to be that result. so this is because of x integration this is because of y integration and then there is 2π/β k because there is a square root and then 3 of them this, this, this. So x, y, z so that is what that is. So now I am now being called upon to evaluate this quantity. So now it is easy. So again remember that what is p_i^2 $p_i^2 = p_{x_i}^2 + p_{y_i}^2 + p_{z_i}^2$

So I am going to rewrite this as dp_{zi} /1/h cubed is outside okay. So there is that then there is this and finally there is the rest of it. I mean the rest of it is simple it is β kappa raise to 3 halves okay. So now how does this work? This is very easy so basically it is just well we have to make sure that the angular momentum is not too high because otherwise this diverges okay. So if I integrate over pzi this is going to look like 2π sorry it is π/square root of a.

So that a is basically β/2m. So it is β/2m and similarly here so this constant also tags along so this one and this one together this and this. So I just have to calculate this but this is the same thing twice over. So what is the coefficient here. So it is again square root of pi/a whole squared and what is a here? a is nothing but you know it is β/2m -β Ω squared/2 kappa. So that is what is. So that is the answer okay. So that is the partition function for 1 particle.

So let me write that out properly. So if I write this out properly it is going to look like

$$Z_1 = \frac{1}{h^3} (\frac{2m\pi}{\beta})^{1/2} (\frac{2\pi}{\beta k})^{3/2} \frac{\pi}{(\frac{\beta}{2m} - \frac{\beta\Omega^2}{2k})}$$

okay. So this is the answer for the partition function for one of the particles and for N particles it is this raise to N. So this is the canonical partition function. So let us try and see what are the other questions that have been asked.

So we answered so they asked us to find canonical partition function we just did. So it is 1 we found it for 1 particle now for N particles you raise it to Nth power. So the next thing we have to find is the average angular momentum. So that is easy because so remember that z is basically it is this integration z e ^ - β H. So if I take dz/dβΩ and put a minus sign I will get an L_z downstairs and then I divide by z.

So this is basically my expectation value of L_z. So it is basically ln so this is nothing but -d/dβΩ lnZ. So I just have to differentiate lnZ with respect to βΩ and put a minus sign. So that is my average value of L_z. So let us do that. So let me do that right here because otherwise I have to flip the slide. So Z is nothing but Z_1^N and lnZ said is N times ln this. So notice that I am going to think of βΩ.

So I am differentiating with respect to Ω and then multiplying by β. So basically I have to differentiate with respect to β. So for that purpose this is irrelevant. So if I take log I will get a whole bunch of things which do not depend on Ω. So I only worry abouπt things which do depend on Ω. So I am going to even ignore this there. So it dimensionally does not make sense but since I am only interested in the derivative with respect to Ω it is okay.

So 2m - β Ω squared/2 kappa. So now if I take the derivative with respect to Ω I get so well I have to differentiate this and then I get -β Ω/kappa okay. Then I put a minus sign and I put a 1/β. So then I get rid of this so this is my L of z average okay. So it is going to be proportional to Ω for small Ω. So you can see that for small Ω so if there is no, if the gas is not rotating then the average angular momentum is 0.

If it is rotating it is for small Ω it is going to be equal to proportional to Ω okay. So I am going to allow you to think about what happens if Ω becomes too large then there is something funny that is going to happen. So I am going to ask you to think about what is the if they have not asked you in this question to think about that. So what I am going to ask you to think about it.

So obviously something funny is going to go on here. So they should have asked that question they have not asked. So but you should think about it. So the other question they have asked is find the average of x squared, y squared and z squared. Well we expect the average of x squared and y squared to be equal but not equal to z squared okay. Because of the nature of the way it is. So I have to calculate the average of z squared separately and average of x squared separately.

But there is a nice symmetry that we can exploit and that is okay you could exploit if we knew how to do the other p quantity. So I am going to have to do it explicitly alright so let us do it anyway. So how do I calculate the average of x squared.

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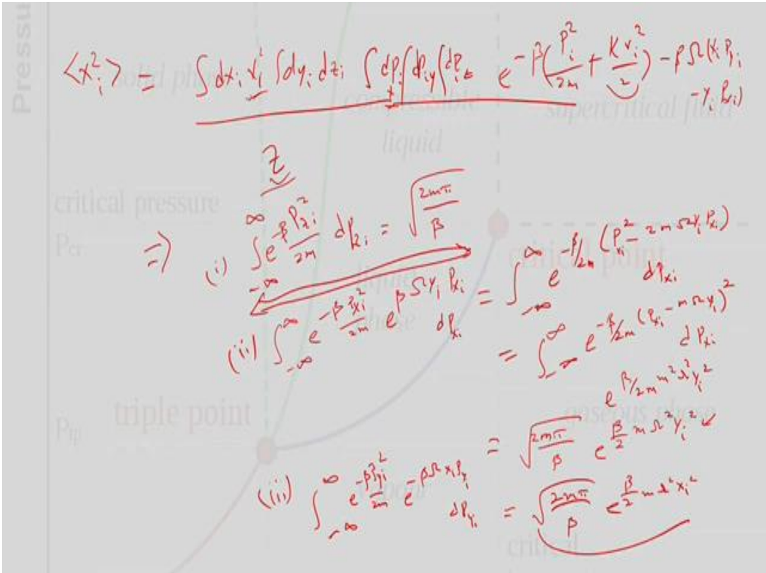

So suppose I am going to calculate the average of x squared. So I have to calculate basically

$$< x_i^2 > = \frac{\int dx_i x_i^2 \int dy_i \int dz_i \int dp_{x_i} \int dp_{y_i} \int dp_{z_i} e^{-\beta(\frac{p_i^2}{2m}+\frac{k}{2}r_i^2)} e^{-\beta\Omega(x_i p_{y_i} - y_i p_{x_i})}}{Z}$$

So you will have to excuse this long expression. So where this Z is the usual canonical partition function without this $x_i^{\,2}$.

So Z is whatever it is without the $x_i^{\,2}$ there. So the question is how do I deal with this? So it is very similar to what we did here except that we have to kind of postpone integrating over you know $x_i^{\,2}$ we kind of integrated over x_i. So we should be doing the p integrations first. So let us do this because I mean it is going to be not so easy to borrow from the earlier result.

So it is going to look like this. So I am going to first do the p integration. So if I do the p integration how does it look like? So the first integration is the one which has only pz. So pzi 2m okay so that is p_{zi} so integrated over all the ps. So this is just going to be square root of 2m π/β okay. So the other pz integration so then you need to do the px integration.

But then px has this linear term as well so you have to deal with that $e^{-\beta(\frac{p_i^2}{2m}+\frac{k}{2}r_i^2)} e^{-\beta\Omega(x_i p_{y_i} - y_i p_{x_i})}$ well this is not a ratio. It is the next calculation so again you have to complete the square and rewrite this in that fashion. So I am going to rewrite this as $\int_{-\infty}^{\infty} e^{-\frac{\beta}{2m}(p_{x_i}^2 - 2m\Omega y_i p_{x_i})} dp_{x_i}$ So this is going to be so pxi – m Ω yi whole squared is going to be this.

And then see this is the completing square so if I square this I get these 2 terms but also I get something which is not there which is the square of vi. So I have to you know cancel that out later on. So in other words I am going to have to rewrite that as β/2m times m squared Ω squared/i squared. So now I have to calculate this and that is nothing but square root of pi 2m pi/β and then I am left with this.

So this was already there so it is 2 times m Ω squared/i squared. So same with the rest of it I mean the last one. So you have

$$\int_{-\infty}^{\infty} e^{-\frac{\beta}{2m}p_{y_i}^2} e^{-\beta\Omega x_i p_{x_i}} dp_{y_i} = \sqrt{\frac{2m\pi}{\beta}}\, e^{\frac{\beta}{2}m\Omega^2 x_i^2}$$

So that is what I get when I integrate over all the ps.

So now I am forced to reckon with x integrations, the x integrations are going to depend upon so there is an xi squared there but there is not any xi squared here. So I will have to deal with that. So I am going to see if look at it here so if I integrate out the yi and the zi so long as the xi does not mix with yi and zi I am safe. So in fact it does not, you see there is no term which has xi times yi or xi times zi.

So I might as well ignore this I might as well not perform the yi and zi integrations because they are going to cancel out coming from here. So the zi so you will have to think about it. So if you do not like all these shortcuts you will have to do it yourself and convince yourself that you can basically the shortcut I am recommending is that you do not do the zi integration or the via integration because the same thing comes in the denominator and xi does not couple because the xi is special.

Because there is an xi squared in the numerator but there is not any in the denominator and so long as xi does not couple to yi or zi. The yi and zi integrations are going to cancel out from the numerator and the denominator. So you might as well not do it. So all you have to do is do the xi integrations and be done with it. So that is what I am going to do now and in order to do that so I am going to use this and the xi part of that okay. So I am going to go to the next slide and write it that way.

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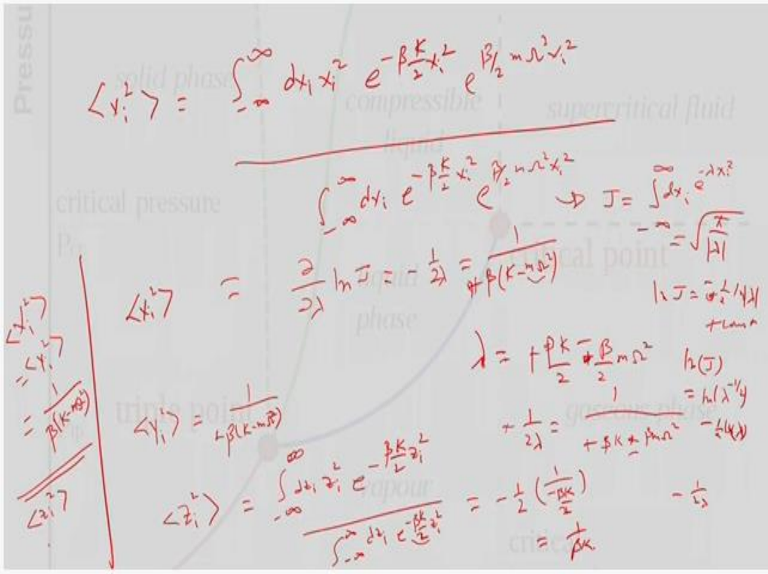

So my xi squared therefore is nothing but integral dxi xi squared times e raise to β. So that comes from there and there is this term in that is all and then I am done because I do not have anything else β/2m e raise to β/2m Ω squared xi squared. So that is all there is to it then without the xi. So this is the average of xi squared. So the question is how do you do this? As usual let me call this something call it some J or something.

So this J has the form $\int_{-\infty}^{\infty} dx_i e^{\lambda x_i^2} = \sqrt{\frac{\pi}{\lambda}}$ and so as far as this is concerned so I can write xi squared average as you know just take the λ derivative of lnJ and you are done. So all I have to do is calculate J. So the λ derivative of lnJ so the lnJ is going to be $\ln J = -\frac{1}{2}\ln\lambda + const$. So the derivative of lnJ with respect to λ is basically $-\frac{1}{2\lambda}$.

So this is $-\frac{1}{2\lambda}$ and so as a result the average so what is λ here? So λ is nothing but so -1/2 λ becomes this is going to look like 1/β kappa - β m Ω squared. So it is going to be $\frac{1}{\beta(k-m\Omega^2)}$. So that is what this is. So we better make sure that it is dimensionally correct at least so you see m Ω squared so β has dimensions of inverse energy and kappa is the spring constant which has dimensions of m Ω squared.

And if I take this here so I get length squared times m Ω squared. So it is going to be x squared times Ω squared which is speed and m times speed squared is energy. So this dimensionally correct. So that is one way of checking after a long calculation it is really disappointing if things do not match dimensionally that is a surefire indication that you have gone wrong somewhere.

And that is an easy way of checking the correctness of your calculation but then do not wait until you have reached the very end. So it is in fact what I did is not advisable. So if you are inexperienced you should periodically check your dimensions in the intermediate steps as well. So then this is as far as x is concerned because x and y are similar this is the same as far as x and y are concerned okay.

So it is the same answer but only thing is now the z does not the same answer as this that is because the z is different okay. So now if it is z so there is no see remember there is no z anywhere else you do not have to worry about any of this. So it is the z squared is as simple as zi squared e raise to β kappa/2 zi squared divided by okay. So no it is the same thing it is just like this with respect to λ okay.

But this is actually -λ okay. So I should have put a mod λ there. The λ is actually the other side sorry I got the sign wrong okay. So it is going to be this sign okay. So it is going to be the other sign okay. So here it is going to be exactly this okay. So differentiating lnJ with respect to λ gave me -1/2 λ. So that is what that is. So it is -1/2 well it is actually sorry it actually becomes plus here there is a so I made mistakes twice.

So it is basically see it is the lnJ is nothing but it is λ raise to -1 half so ln of that. So it is -1 half ln of λ okay so that was correct. So now I am going to have to calculate this as 1/2 λ and this is my λ. So it is going to be 1/-β kappa/2. So this is going to look like 1/β kappa okay. So sorry this was plus then okay. So that makes sense now. So it has to when Ω is 0 they have to be all equal okay.

So I am sorry for the sloppiness but so if you do it properly you will get this. So now let me summarize so average value of x squared is same as average value of y squared which is same as 1/β times kappa - m Ω squared and whereas the average value of zi squared is as if there is no Ω okay. So yeah now it makes sense okay. So that answers all the questions that are asked here.

And so you can see that you know some of these calculations can be a little tedious even though it is straightforward but unless you do it yourself so and one of the highlights of this calculations that I have shown you here is that I have done everything by hand you know I have not used any computer or any software. In fact that is also not advisable. So nowadays you have software which does all this.

So it is actually a waste of effort and waste of time to do it this way. So it is better for you to learn some software some symbolic algebra packages like Mathematica and you just type in your integrals there and you get the answer. So I am going to stop here and continue with my tutorial questions in the next hour.