

Introduction To Statistical Mechanics
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Lecture - 19
Tutorial - I

Okay so what I have decided to do now is to solve some tutorial type of problems that means I want to train you to think about the concepts that I have been teaching you in this course through examples, detailed worked out examples. So it is possible that some of you would have found the course I mean the actual lectures a bit fast in terms of the pace of presentation. So maybe many you know intermediate steps were missing and they were implied and you probably had a difficult time in places to fill in those missing steps.

So it is important nevertheless even if you are confident of all those steps it is important for you to test your understanding of the concepts by working out some of the examples that I am going to be presenting right now. So these examples you know go to the heart of the subject and they kind of make sure that you understand the concepts at the end of the day. So you can confidently claim you understand statistical mechanics okay.

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Tutorials

1. Imagine $2N$ labelled sites on a line. At each site there is a spin that can point up or down. If it points up its energy is $+1$ and if it points down its energy is -1 . Find the entropy of the system if the total energy is 0 . Also find the canonical partition function at temperature T and the average energy.

Ans.

The total energy is $U = \sum_{i=1}^{2N} \sigma_i$ where $\sigma_i = \pm 1$. The total energy is zero if N sites are up and the remaining are down. We just have to find the number of ways in which N sites can be populated with up spins from a total number of $2N$ sites. The answer is

$$e^{S(U=0)} = \frac{(2N)!}{N!N!}$$

Hence $S(U=0) = \text{Log} \left(\frac{(2N)!}{N!N!} \right)$

So imagine you have $2N$ labelled sites on a line. So the idea is that I am thinking of a straight line here and there is a lattice for convenience sake I am going to assume that there are even number of sites. So the number of sites are $2N$ dot, dot, dot, dot $2N$ so on each site there is a

spin which can be up or down. So for example I can have a situation like this some can be pointing up some can be pointing down.

So the idea is that if a spin points up its energy is ϵ , if it points down its energy is $-\epsilon$. So for example if in this configuration the energy is one is up the other is down. So you just count how many ups are there and you subtract it with the number of downs. So you see there is one more down than up. So that total energy is $-\epsilon$ here okay. So in general it is going to be this.

So the total energy is going to be the number of ups minus the number of downs. So the total energy is 0. So the question is find the entropy of the system if the total energy is 0 and also find the canonical partition function at temperature T and average energy at that temperature okay. So now let us think about the entropy of the system. So if the total energy is 0, what is the entropy of the system?

So we have to calculate the number of ways in which the total energy of the system can be 0. So the number of ways in which the total energy can be 0, if there are as many sites which have up spin as there are number of sites that have down spin. So the question is how many ways can you accomplish that? So the answer is clearly you just have to look at the combination because the sites are all labelled.

Remember that the sites have specific labels so you can tell each site apart from the others. So as I said you just have to count the number of combinations of selecting N sites from the total number of sites which is $2N$. So you can choose to assign those sites with the up spins. So then you are forced to make the others down spin. So you select N of them to be up spin and the others to down spin.

So the question is how many ways can you select N sites out of $2N$ sites? So the answer is the combination of $2N$ taken and at a time okay the binomial coefficient. So it is $2N$ factorial or N factorial squared. So now this is the number of ways in which you can select those sites. So now the entropy is defined as the log of this number and so that is the entropy. So that answers the question.

So I hope this is clear to you because this is one of the fundamental concepts in the subject the entropy concept. So if you are having difficulty calculating entropy for such simple systems then you should revisit some of these issues and learn them properly until you are able to answer these questions on your own okay. So the next question is find the canonical partition function at a temperature T and the average energy okay?

So if the system is allowed to exchange energy with the surroundings then its energy is not going to be fixed. So its energy is not going to be fixed and so all you can do is find the average energy of the system. So the question is how do you do that?

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The canonical partition function is,

$$Z = \text{Tr}(e^{-\beta U}) = \text{Tr}\left(e^{-\beta \sum_{i=1}^{2N} \sigma_i}\right) = (2 \cosh(\beta))^{2N}$$

The average energy is,

$$\langle U \rangle = -\frac{\partial}{\partial \beta} \ln(Z) = -2N \tanh(\beta)$$

2. Imagine labelled sites on the corners of a cube as shown. Imagine I place identical charges at the corners. Find the entropy of the system as a function of the number of charges and total electrostatic potential energy of the system.

So the way to find the canonical partition function is to take the trace of $e^{-\beta U}$ in terms of the microstates. So remember the microstates are the configurations of all the σ_i s. So now you trace out over all the microstates and we do it in the usual way you know that you can write this as the product of $e^{-\beta \sigma_i}$ and then you have to trace over all of them.

So that means you have to sum over all the configurations and I have showed you earlier in the lectures that it is possible to interchange the product in the sum and you can interchange it in this fashion and then you take the sum over a $\sigma_i = \pm 1$ $e^{-\beta \sigma_i}$. So this sum is precisely twice cosine hyperbolic β and the product if you take the product over $2N$ sites. So it is like multiplying twice $\cosh \beta$ with itself $2N$ times.

So that is basically raising $2 \cosh \beta$ to the power $2N$. So now the average energy is given by the standard relation in canonical formalism as the derivative of $\log Z$ with respect to β with a minus sign and so as I said you get this result okay. So you can examine various limiting cases and convince yourself that this makes sense, suppose β is very small that means the temperature is very large.

So if temperature is very large you expect a line of randomization of the spin so you expect roughly equal number to point up as they point down. So when β is small you can see the average energy tends to 0. But then conversely if β is very large so temperature is very small so you can expect the system to be in the ground state that means you expect all the spins to point down.

So that means you expect the energy to be $-1, -1, -1$ for all the spins. So as a result the total energy you expect it to be $-2N$. So if β tends to infinity which is temperature tends to 0. So this becomes $\tanh \infty$ is 1 and so as a result the average energy is $-2N$ at very low temperatures and it is 0 at very high temperature so it is correct. So we can we are able to reconcile it with our intuition and so it makes sense okay.

So that is the first problem regarding the concept of entropy and to some extent the canonical formalism also appears in this example all right. So now the next example is slightly more challenging and it relates to finding again the entropy of the system but now the problem is as follows, imagine that there is a cube here where the corners of the cube at the corners of the cube so remember there 8 corners.

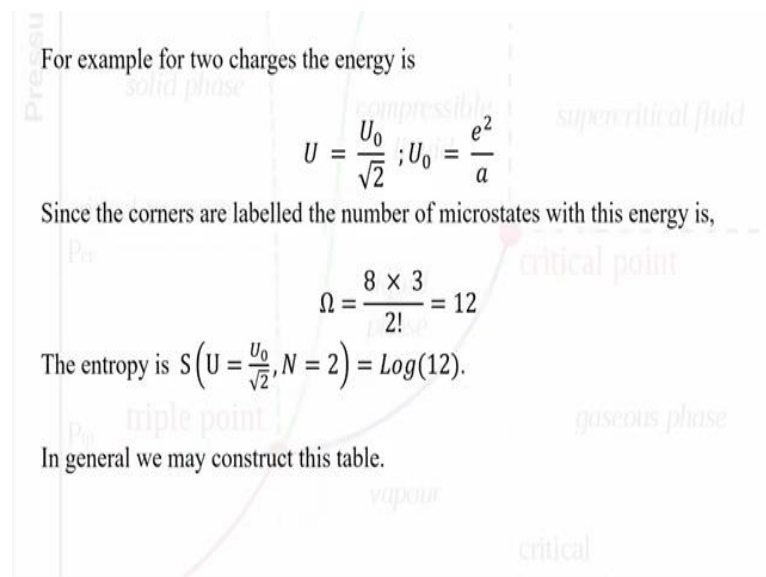
So at each corner of the cube there is a charge that is placed and so the question is I want to find the so I am not going to tell you how many charges there are. So you can have a system with variable number of charges. So you can start with 1 charge, 2 charges and a maximum of 8 charges. So you can have all 8 corners occupied and of course if you are going to assume that the corners are all labelled.

So that mean I know which corner is which I know this is corner number 1, corner number 2, corner number 3, corner number 4 and that way. I mean I can kind of label them in some way so the corners are all labelled but the charges are identical so I am going to ask myself so if I

have say 2 charges so the energy of the system is by definition the electrostatic potential energy of the systems.

So the charges repel each other and they have an electrostatic repulsion and that is going to be the energy of the system. So I am going to ask myself as a function of the energy of the system and the number of charges so if I tell you the energy and tell you the number of charges I want to know how many ways there are of distributing these charges at these corners in such a way that the energy is that particular value. So that is going to be the number of microstates and the log of that is going to be the entropy of the system. The question is how do I calculate this?

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For example for two charges the energy is

$$U = \frac{U_0}{\sqrt{2}}; U_0 = \frac{e^2}{a}$$

Since the corners are labelled the number of microstates with this energy is,

$$\Omega = \frac{8 \times 3}{2!} = 12$$

The entropy is $S\left(U = \frac{U_0}{\sqrt{2}}, N = 2\right) = \text{Log}(12)$.

In general we may construct this table.

So take for example let us start with a simple example. So imagine that there are 2 charges okay so there are 2 charges. So if there 2 charges you can you know either choose to you know place them here and here for example. So that means you can choose to place them at sites 2 and 3 or you know equivalently 2 and this or 1 and this. So it could be any of these so along one of the edges.

So that means the 2 charges are on the edges. So that way you can get an energy which is this one okay so that is called U_0 so and a is the side of the cube. So you can get an energy of that form e^2/r but then so that is one of the possible energies. So the other possible energy is if you decide to place them here and there for example. So you can place them here and there and you can get e^2 by see this distance is what square root of 2 times a .

So the number of microstates for example with the energy which is this. So if this is the energy then if there are 2 charges the number of microstates is 12. So you can imagine that there are 12 ways in which you can select this then you can so that 12 ways you can select pairs of corners you can just figure that out yourselves okay. So it is easy to convince yourself that 12 ways of doing it and the entropy is just log of that.

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$U = (2 + \frac{1}{\sqrt{2}})U_0 = U_0 + U_0 + U_0/\sqrt{2}$

Number of particles	$U = \frac{2}{3}U_0$	$U = U_0$	$U = \frac{4}{3}U_0$	$U = \frac{5}{6}U_0$	$U = \frac{2}{3}U_0$	$U = \frac{1}{2}U_0$	$U = \frac{1}{3}U_0$	$U = \frac{1}{6}U_0$	$U = \frac{1}{12}U_0$	$U = \frac{1}{24}U_0$	$U = \frac{1}{48}U_0$	$U = \frac{1}{96}U_0$
2	$\Omega = 12$	$\Omega = 12$	$\Omega = 4$	$\Omega = 0$	$\Omega = 0$	$\Omega = 0$	$\Omega = 0$	$\Omega = 0$	$\Omega = 0$	$\Omega = 0$	$\Omega = 0$	$\Omega = 0$
3	$\Omega = 0$	$\Omega = 0$	$\Omega = 0$	$\Omega = 24$	$\Omega = 8$	$\Omega = 24$	$\Omega = 0$	$\Omega = 0$	$\Omega = 0$	$\Omega = 0$	$\Omega = 0$	$\Omega = 0$
4	$\Omega = 0$	$\Omega = 0$	$\Omega = 0$	$\Omega = 0$	$\Omega = 0$	$\Omega = 6$	$\Omega = 24$	$\Omega = 8$	$\Omega = 24$	$\Omega = 2$	$\Omega = 6$	$\Omega = 0$
5	$\Omega = 0$	$\Omega = 0$	$\Omega = 0$	$\Omega = 24$	$\Omega = 8$	$\Omega = 24$	$\Omega = 0$	$\Omega = 0$	$\Omega = 0$	$\Omega = 0$	$\Omega = 0$	$\Omega = 0$
6	$\Omega = 12$	$\Omega = 12$	$\Omega = 4$	$\Omega = 0$	$\Omega = 0$	$\Omega = 0$	$\Omega = 0$	$\Omega = 0$	$\Omega = 0$	$\Omega = 0$	$\Omega = 0$	$\Omega = 0$

When all the sites are occupied the potential energy is a maximum. This is given by,

$$U_{max} = U_0 (12 + \sqrt{\frac{2}{3}} + \frac{11}{\sqrt{2}} + \sqrt{3}).$$

The number of microstates with energy U and number of N is same as

The number of microstates with energy $U_{max} - U$ and number of particles $8 - N$. The entropy is given by $S = \log(\Omega)$.

Handwritten notes:
 $U_5 = U_0 - U_3$
 $U_0 + \frac{U_0}{\sqrt{2}} + \frac{U_0}{\sqrt{2}}$
 $U_0 - \frac{U_0}{\sqrt{2}}$

And so the table is as follows and this is the table and so you see the table says the of course see I have purposely omitted 1 charge I mean if there is 1 charge there is no fun. Because the potential energy there you need a minimum of 2 charges. But I have also interestingly omitted 7 and 8 see 0 charge I have omitted, 1 charge I have omitted. So if there is only 1 charge in the system it is uninteresting, 0 is even more uninteresting.

But then the question is why have I omitted 7 charges and 8 charges from the table? See that is because there is something called particle-hole symmetry that means that the so you can think of 7 charges as 1 positive charge. So you can think of you know a missing charge as a whole you know just like you doing semiconductors. So if you populate that corners with all 8 charges and you remove 1 of them so you get actually 7 negative charges.

But that is equivalent for all practical purposes with 1 positive charge. So as a result you know that because so combinatorially it is identical to studying 1 negative charge, 1 positive charge has the same component **or** as 1 negative charge. So 7 is uninteresting because it corresponds to 1 I mean it is analogues to 1 because 7 is just absence of 1 it is absence of 1 charge from a cube where all the corners are occupied by charges.

So that is equivalent to 1 charge. So as a result I am omitted both 7 and 8 and 0 and 1 are obvious why I have omitted them. So now as a result I am going to start populating this table starting from the number of charges with number of charges equals 2, number of charges equals 3 and number of charges equals 4 and then rapidly after 4 I have my work is

significantly simplified because when it is the number of charges is 5 remember that 5 is same as the combinatorics of 5 charges is same as $8 - 5$ which is 3.

So I do not have to populate this row at all. I just copy paste the row containing 3 charges and fill it with the 5 charges and I take the row that I have populated for the number of charges equals 2 and I copy paste it on the row containing 6 charges because $8 - 6$ is 2. So all I have to do now is populate these 3 rows okay this up to 4. So long as I do this then I am done. So the question is how do I do that?

So now I have to list all the possible energies that are seen when there are 2 charges. So like I told you that if they have 2 charges then only 3 possible energies one is U_0 which is e^2/a and the other is $U_0/\sqrt{2}$ and they are diagonally opposite and $U_0/\sqrt{3}$ when there are when you know there is as far as part as they can possibly be. So now you ask yourself how many ways there are in which you can achieve an energy of U_0 ?

That is going to be 12. In fact I wrote a small program which does this in language called Mathematica and it is something that you should do yourself. So I am not going to constrain you to any specific language so you can write your own code and come up with these results. So it is just question of combinatorics. So you have to it is better to write a computer program to turn out these numbers rather than doing it by hand.

Because firstly it is tedious and secondly and because it is tedious there is a chance you will make mistakes. However if you write a program and you test your validity of your program using simple examples if it comes out right then it is unlikely that it is going to be wrong for you know more complicated situations. So that is typically how people do it. So they are test it out for some obvious limiting cases and then cross their fingers and hope for the best.

Most typically it is now going to go wrong most of the time if you are you know if you are a moderately experienced programmer okay. So this is 12 is the number of ways in which you can rearrange the microstates to get energy $U_0/\sqrt{2}$ and it is 12 is also the number of ways you can achieve an energy of U_0 and the only 4 ways in which you can achieve an energy of $U_0/\sqrt{3}$.

And all the other columns are empty because there is no way you can get any of these other energies that I have mentioned there okay. So what about the other energy so I am talking about what about the other number of particles. So there are 3 particles so if the 3 particles then the possible energies start off with this one which is I hope you can see this. This is nothing but $U = 2 + 1 \text{ over square root of } 2 \text{ times } U_0$.

So where does this come from you can easily guess where this comes from this is the $U_0 + U_0 + U_0 \text{ over square root of } 2$. So that implies that you know there is a charge at one location is charge distance a part so which means that there is a potential energy of U_0 and then there is another that is diagonally apart. So you see that there is a pairwise interaction okay. So if you have a situation like this.

So this pair has potential energy U_0 , this pair has potential energy U_0 and this pair has potential energy $U_0/\text{square root of } 2$. So put together that is the total potential energy okay that is this example okay. So like that you start populating so if that is the energy then there are 24 ways of achieving back. So that is going to be very painful to list all of them. So that is the reason why you should write a program to list them.

So similarly you start getting all these other possible energies this $U_0/\text{square root of } 2 + U_0/\text{square root of } 2 + U_0/\text{square root of } 2$. So that is 3 times $U_0/\text{square root of } 2$. So there are 8 ways of doing that. And similarly you will get one more where this diagonal thing is $1/\text{square root of } 3$ that is you know the other end of the cube diagonally. So there also you get 24 ways of doing it and all the other energies are impossible for 3 number of charges.

So now again if you have 4 charges then again the number of you know all different energies are possible and now there are many more. If there are 4 charges you have so many more energies that are possible and they are all listed here and it is $4 + \text{square root of } 2 \text{ times } U_0$ and $U_0 \text{ times } 2 + 3/\text{square root of } 2 + 1/\text{square root of } 3$ and there is this possibility which says that it is $3 + 3 \text{ over square root of } 2 \text{ times } U_0$ then $3 + \text{square root of } 2 \text{ over } 1$.

So these are all kinds of possible energy so you should look this up. So we have 1, 2, 3, 4, 5, 6 possible energies when the number of particles is 4 and the number of ways in which you can achieve see this energy which is $4 + \text{square root of } 2$ is 6 and you can achieve you know the energy which is $2 + \text{square root of } 3/2 + 1/\text{square root of } 3$ that energy is achievable in 24

ways. So like that you populate this table by you know preferably by writing a program that is how I did it.

And I used this software called Mathematica which is very useful for doing this type of calculations and then I told you for 5 and 6 I did not do anything. I just copy pasted the 3 row into row 5 and of course here are the you have to take this with a grain of salt this is not really the energy it is the it is actually the maximum energy minus U. So the maximum energy is when all the 8 corners are occupied.

So if you have you know 5 charges, the energy is not the same as 3 charges. So if you have so 5 charges it is the same as the 8 charges – 3 charges you see that is what I am saying. So the maximum possible energy so minus this okay. So however the omegas are the same okay. The number of ways in which you can populate those locations are identical to 5 is identical to 3 as far as omega is concerned.

So 6 is identical to 2. So that is how you do it and so this is a moderately challenging example which I feel that you should learn to do properly. So that you will understand how to so the log of omega is entropy. So you will be able to understand you know the combinatorial basis for entropy okay.

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Euler Maclaurin formula

Euler Maclaurin formula tells us how to replace a discrete sum by an integral which are typically easier to evaluate. The version we employed in this course is,

$$\sum_{i=0}^{\infty} f(i) \approx \int_0^{\infty} f(x) dx + \frac{1}{2} f(0) - \frac{1}{12} f'(0) + \frac{1}{720} f'''(0) - \dots$$

We could use Fourier analysis to prove this. Write the Fourier transform and its inverse as follows,

$$f(x) = \int_{-\infty}^{\infty} e^{ikx} g(k) \frac{dk}{2\pi}; \text{ where } g(k) = \int_{-\infty}^{\infty} e^{-ikx} f(x) dx$$

Handwritten notes on the slide include:
 $\int dx e^{ikx} = \frac{1}{ik}$
 $\sum_{n=-\infty}^{\infty} f(n) = \int_{-\infty}^{\infty} \frac{dx}{2\pi} \sum_{n=-\infty}^{\infty} e^{ikn} f(x) = \int_{-\infty}^{\infty} \frac{dx}{2\pi} \frac{1}{1 - e^{ikx}} f(x)$

So the other topic that I kind of I have used frequently but maybe not explained it is derivation all that well. I explained somewhere once but it was not fully convincing. So I am going to explain it again properly and this is called Euler Maclaurin formula. So the Euler

Maclaurin formula is frequently used in physics although many times authors and you know teachers do not call it that.

Because in the maths community it is known as Euler Maclaurin formula but we kind of use it without calling it anything specific. But it is important to know that you know that there is a systematic way of deriving it is not some hand waving approximation but there is a you know there is a proper way of understanding how this comes about. And so it so happens that there is a series which tells you so Euler Maclaurin formula is basically a method which enables you to replace a discrete sum by an integration.

So typically because discrete sums are harder to do than integrations. So which seems odd but then you know think about look if it is a finite sum then it is by definition simple. But I am talking about an infinite sum. So infinite sum that actually limits of finite sums. So in those limits can be hard to calculate. So as a result however if it is an integration many times there are lots of tricks you can use to analytically evaluate integrals.

But the fewer tricks you can use to evaluate infinite sums all right. So it is nice to know that you can convert infinite sum to a integral and the way you do that is through the Euler Maclaurin formula. So the question is how do you do this? So the way you do that firstly I am going to state the Euler Maclaurin formula. So Euler Maclaurin formula states there is a summation of f_i over from $i = 0$ to infinity is the same as integrating from replacing i by x and integrating x from 0 to infinity well we have kind of most of the time stopped here we have equated this to this.

But in fact that is not strictly true that there are additional terms and if you can convince yourself that typically this is always there but if you can convince yourself that these can be neglected then this has a lot of use as you can directly use this okay. So but then if you cannot convince yourself that these are small then you will have to evaluate them. But then keep in mind that these functions and their derivatives are to be evaluated at exactly 1 point.

So it is not going to be that difficult and keep in mind that these coefficients are rapidly diminishing and there is a good chance that you won't be you know going terribly wrong if you truncate this series after a certain point all right. So the question is how do you derive

this series? So this is exact. So I mean if you continue forever it is exact. So the question is how do you prove this.

So my method of course is I mean there many ways of doing this in some of the maths books you will find that this is a special case of what is called the Darboux formula which is just obtained by integration by parts. So I mean those may be probably more mathematically rigorous. But I am going to use a method which is simpler but probably not very rigorous but I feel that physics audience will appreciate this derivation a lot more than they would some more rigorous derivation.

But then you should also learn those other derivations which are favoured by mathematics people. So my derivation is as follows, so I am going to write f of x in terms of its Fourier transform. So and then this makes sense only if I know how to calculate g given f . So it so happens that you can invert the Fourier transform in this fashion. So this is called the Fourier transform and inverse Fourier transform pair. So this is well known in physics and frequently used.

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$$\sum_{i=0}^N f(i) = \int_{-\infty}^{\infty} \cos\left(\frac{kN}{2}\right) \csc\left(\frac{k}{2}\right) \sin\left(\frac{1}{2}(N+1)k\right) g(k) \frac{dk}{2\pi} + i \int_{-\infty}^{\infty} \csc\left(\frac{k}{2}\right) \sin\left(\frac{kN}{2}\right) \sin\left(\frac{1}{2}(N+1)k\right) g(k) \frac{dk}{2\pi}$$

Taking the limit $N \rightarrow \infty$ we get $\left(\cos\left(\frac{kN}{2}\right)\right)^2 = \sin\left(\frac{kN}{2}\right)^2 = \frac{1}{2} \sin\left(\frac{kN}{2}\right) \cos\left(\frac{kN}{2}\right) = 0$

$$\sum_{i=0}^{\infty} f(i) = \frac{1}{2} \int_{-\infty}^{\infty} g(k) \frac{dk}{2\pi} + \frac{i}{2} \int_{-\infty}^{\infty} \csc\left(\frac{k}{2}\right) \cos\left(\frac{k}{2}\right) g(k) \frac{dk}{2\pi} = \frac{1}{2} \int_{-\infty}^{\infty} g(k) \frac{dk}{2\pi} + \frac{i}{2} \int_{-\infty}^{\infty} \cot\left(\frac{k}{2}\right) g(k) \frac{dk}{2\pi}$$

Note that,

$$f(0) = \int_{-\infty}^{\infty} g(k) \frac{dk}{2\pi} \cdot \int_0^{\infty} f(x) dx = - \int_{-\infty}^{\infty} \frac{1}{ik} g(k) \frac{dk}{2\pi}$$

$$f'(0) = \int_{-\infty}^{\infty} ik g(k) \frac{dk}{2\pi} ; f'''(0) = \int_{-\infty}^{\infty} (ik)^3 g(k) \frac{dk}{2\pi}$$

Handwritten notes on the right side of the slide include:

- $\sin\left(\frac{1}{2}(N+1)k\right) = \sin\left(\frac{Nk}{2}\right) \cos\left(\frac{k}{2}\right) + \cos\left(\frac{Nk}{2}\right) \sin\left(\frac{k}{2}\right)$
- $\sin\left(\frac{Nk}{2}\right) \cos\left(\frac{k}{2}\right) = \frac{1}{2} \left[\sin\left(\frac{(N+1)k}{2}\right) + \sin\left(\frac{(N-1)k}{2}\right) \right]$
- $\cos\left(\frac{Nk}{2}\right) \sin\left(\frac{k}{2}\right) = \frac{1}{2} \left[\sin\left(\frac{(N+1)k}{2}\right) - \sin\left(\frac{(N-1)k}{2}\right) \right]$

So I am going to try and see if I can rewrite so okay I skipped a slide okay. So look I am going to replace x by i . So you will have to excuse me or maybe I will replace it by m . So f of m is going to be e raise to ikm $g(k) dk$ then I am going to sum over all the m s from 0 to infinity. So now notice that the summation of m of e raise to ikm is nothing but okay from 0 to infinity is 1 over $1 - e$ raise to ik .

So I can kind of rewrite this in this fashion okay. I am going to first sum up to N okay. So I am going to sum up to N and then integrate later. So I have replaced x by m and I have summed up to N okay. So I got this answer so because it is e raised to i thing. So I can replace rewrite in terms of its real and imaginary parts. But now this is important because I cannot really sum up to infinity because remember that the geometric series converges only if the mod of r is < 1 . So if it is r raised to m and sum over m from 0 to infinity it converges only if $|r| < 1$.

But here in this example r is e^{ik} where $|r|$ is exactly 1. So I cannot really sum up to infinity so what I should do is sum up to a certain value for N and then finally take some kind of a limit as N tends to infinity. So now this limit strictly speaking does not exist in the mathematical sense but we use our physics intuition and say that you see when N tends to infinity we kind of intuitively argue that cosine squared kind of becomes half.

Because a cosine squared $kN/2$ see cosine itself oscillates rapidly. So it oscillates rapidly between negative and positive values equally. So when N becomes infinity cosine $kN/2$ averages out to 0 okay. So because it is positive as frequently as it is negative and when N tends to infinity it kind of rapidly you know flips between being 1 and -1. So on an average it is always 0. But then if it is cosine squared it is between 0 and 1 most of the time.

It is always between 0 and 1 and it flips between 0 and 1 so rapidly that its value is the average between 0 and 1 which is 1/2. So same with so in case of $\sin \cos$ it is nothing but you know 1/2 of \sin of kN itself and I told you that because \sin of kN oscillates rapidly between -1 and 1 its average is out to 0. So now with those ideas so I am going to use the trigonometric identity here and write this as you know $\sin \cos$.

So I am going to pull this $\sin N k/2$ out because there is a \cos there and so on. So I have done all that and using this idea and using trigonometric identities. So I am going to write \sin of 1/2 of $N + 1 k$ the \sin of $N k/2 \cos k/2 + \cos Nk/2 \sin k/2$ okay. So I am going to write all this. So I am going to write $\sin \cos + \cos \sin$ okay. So if I do that and I use all these identities I end up getting this equation okay.

So that is one idea which I am going to give under my thumb. So now also note that if I take this formula and put $x = 0$ again an integration which is this. So if I take f of x and put $x = 0$ I

get this. Then if I integrate f of x take this integrate f of x from 0 to infinity because it is so integral of $dx e^{ikx}$ from 0 to infinity is basically 1 over ik with a minus sign because at infinity it oscillates and becomes 0.

So that is our physicists way of doing things. So you get this result so $-1/ik$ times the rest of it. So same with if I differentiate with respect to x and put equal to 0 that is easier I get this. I differentiate thrice I get this. So I am going to keep this also under my thumb and now I am going to do this.

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$$\cot\left(\frac{k}{2}\right) \approx \frac{2}{k} - \frac{k}{6} - \frac{k^3}{360}$$

$$\sum_{i=0}^{\infty} f(i) = \frac{1}{2}f(0) + \frac{i}{2} \int_{-\infty}^{\infty} \left(\frac{2}{k} - \frac{k}{6} - \frac{k^3}{360}\right) g(k) \frac{dk}{2\pi} =$$

$$\frac{1}{2}f(0) + \int_0^{\infty} f(x)dx - \frac{1}{12}f'(0) + \frac{1}{720}f'''(0) - \dots$$

I have to apologize the slides got flipped this should have come later okay. So now notice that there is a cotangent well yeah there is a cotangent here. So this plus this adds up and becomes this. Because this is nothing but cotangent okay. So it becomes this. So now notice that this is nothing but $f(0)/2$. So now I have to manipulate this. So I am going to expand cotangent $k/2$ in powers of k .

So when I do that I get this series okay. So I am going to insert that series here and then when I do that you see lo and behold I start getting that terms that I was staring at earlier namely I start I get this then the case you know when I do it this way. So this becomes you know this result there is a k downstairs, there is a k downstairs here also. So it becomes this and I get these other terms. So you see so the sum over all the is from $i = 0$ to infinity becomes this Euler Maclaurin series.

So it becomes this integration. So it becomes this Euler Maclaurin series okay. So it is becomes this. So it is this plus this plus this plus this and so on. So I hope you are convinced by this derivation. So this is an important formula that is used again and again in physics and you know it is worthwhile to know how it was derived okay.

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Saddle point method

Imagine I want to calculate the integral

$$I(N) = \int_{x_1}^{x_2} dx g(x) e^{N f(x)}$$

where $N \rightarrow \infty$ is large. The idea is to try and write a series for $I(N)$ in powers of $\frac{1}{N}$ when it is assumed that the function $f(x)$ has a maximum at $x_1 < x_0 < x_2$. This means,

$$f'(x_0) = 0, \quad f''(x_0) < 0$$

The contribution to $I(N)$ is dominated by contributions from x close to x_0 . Hence we may write,

$$I(N) \approx g(x_0) \int_{x_1}^{x_2} dx e^{N (f(x_0) + \frac{1}{2}(x-x_0)^2 f''(x_0) + \dots)}$$

Set $\sqrt{N}(x - x_0) = y$

The other thing that I have used extensively in this course which I can probably did not explain to very well and but then I am going to try now. This is called the Saddle point method. So the Saddle point method of course again this is a bit of special case which it does not do justice to the word saddle point. In this case it is merely a maximum is not even an extremum is a maximum let alone a saddle point.

So saddle point comes about if you are trying to do integrations over complex functions of a complex variable. But in this case I am only going to restrict myself to integrations over real variables real functions over a real variable in which case there is no saddle point there is just a maximum. So now imagine that I want to calculate this integration over so there is an integrand which is g of x times e raise to N .

So this N is very large. So the idea is that N is huge then I want to calculate this integration. I want to perform this integration from between x_1 and x_2 when N is large. So the idea is to write a series for I of N in powers of $1/N$ where it is assumed that f of x has a maximum. So the idea is that let us imagine that there is an f of x which has a maximum between x_1 and x_2 okay. So it goes through a maximum.

So I want to calculate this integration when it goes through a maximum and N is very large. So that is when the saddle point is very useful. So it is clear that the maximum contribution to this integration comes from regions where the integrand is very large. So the integrand is because N itself is huge. So the integrand is dominated by the regions where $f(x)$ goes through a maximum near the peak.

So since I have denoted choose to denote the location where the function f of x peaks has x_0 . So I am going to therefore conclude that its first derivative is 0 because it is a maximum, second derivative is a negative because again it is a maximum not a minimum. So then I can Taylor series expand f of x around x_0 and I end up getting this result all right. So I get this result which is basically this Taylor series.

So the first derivative is absent because it is a maximum and notice that because g of x is assumed to be regular in this interval and you know the dominant contribution clearly comes from this integrand here. So I have chosen to replace this by x_0 and pull it outside. So now I am going to do a change of variables I am going to set y to be this quantity. Because the exponent involves $x - x_0$. So I am going to set that equal to y . So then I can replace just through change of variables I can do the integration over y instead of x .

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The image shows a handwritten derivation of the saddle point approximation. It starts with the integral $I(N) \approx \frac{g(x_0)}{\sqrt{N}} e^{N f(x_0)} \int_{y_1}^{y_2} dy e^{\frac{1}{2} y^2 f''(x_0)}$. Red arrows indicate the substitution $y = \sqrt{N}(x - x_0)$. The limits $y_1 = \sqrt{N}(x_1 - x_0) \rightarrow -\infty$ and $y_2 = \sqrt{N}(x_2 - x_0) \rightarrow \infty$ are shown. The integral is then transformed to $I(N) \approx \frac{g(x_0)}{\sqrt{N}} e^{N f(x_0)} \int_{-\infty}^{\infty} dy e^{\frac{1}{2} y^2 f''(x_0)}$. The final result is $I(N) \approx \frac{g(x_0)}{\sqrt{N}} e^{N f(x_0)} \sqrt{\frac{2\pi}{|f''(x_0)|}}$. At the bottom, the logarithm of the integral is given as $\ln I(N) = N f(x_0) + \ln \left(\frac{g(x_0)}{\sqrt{N}} \sqrt{\frac{2\pi}{|f''(x_0)|}} \right)$. The background features a phase diagram with labels for solid, liquid, and gaseous phases, and critical and triple points.

$$I(N) \approx \frac{g(x_0)}{\sqrt{N}} e^{N f(x_0)} \int_{y_1}^{y_2} dy e^{\frac{1}{2} y^2 f''(x_0)}$$

where,
 $y_1 = \sqrt{N}(x_1 - x_0) \rightarrow -\infty ; y_2 = \sqrt{N}(x_2 - x_0) \rightarrow \infty$

Hence,

$$I(N) \approx \frac{g(x_0)}{\sqrt{N}} e^{N f(x_0)} \int_{-\infty}^{\infty} dy e^{\frac{1}{2} y^2 f''(x_0)} = \frac{g(x_0)}{\sqrt{N}} e^{N f(x_0)} \sqrt{\frac{2\pi}{|f''(x_0)|}}$$

$$\ln I(N) = N f(x_0) + \ln \left(\frac{g(x_0)}{\sqrt{N}} \sqrt{\frac{2\pi}{|f''(x_0)|}} \right)$$

So I am going to integrate over y and from y_1 to y_2 okay. So where y_1 is this and y_2 is this, notice that x_1 is less than so x_1 is here, x_0 is here okay and x_2 is there. So that means x_0 is between x_1 and x_2 . So because of that you see y_1 tends to $-\infty$ because N is huge,

remember that N is huge. So if N is huge and this is negative. So y_1 tends to be $-\infty$ and also because N is huge and this is greater than 0, x_2 is greater than x_0 .

So this is more than 0. So this is positive. So y_2 tends to $+\infty$. So as a result I am at liberty to approximate this by $-\infty$ and $+\infty$ and this becomes approximately so notice that this is negative. So this makes perfect sense and then I am going to be able to write this in this fashion. So this is the saddle point, so you see that for the most part I have so if I take \log of I_N this is going to be N times f of x_0 plus a whole bunch of other things which kind of you can sort of ignore.

Because well the only reason why you should not ignore it is for dimensional reasons because this may have some dimensions which is make but this is dimensionless. So otherwise for the most part you can ignore this. So notice that N is very large. So this is roughly ignorable unless you have dimensional issues then only you should take this into account alright. So this is basically the you know the baby version or the real version of saddle point as opposed to the complex version.

So the real saddle well the actual saddle point occurs in a situation where you are integrating on the complex plane over functions of a complex variable. But here it is an order saddle point it is a maximum but it is the ideas are similar. So the whole idea is to kind of replace the exponent of the integrand by its maximum value or near the maximum value. So that you can perform the integration as a Gaussian and then you just live with that okay.

So that was the tutorial for today. So hopefully you will join me for some of the other tutorials that I am going to discuss. So I am going to start explaining to you various other concepts through examples. So that way you will be able to better grasp the lectures that you have been listening to. Thank you. Hope to see you next time.