

Statistical Mechanics
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Lecture - 26
Example of Microcanonical Ensemble - Ultra-Relativistic Gas

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Microcanonical Ensemble

- * Paramagnet to ferromagnet transition
- * Ideal gas $\chi = \sum_i \frac{p_i^2}{2m} \rightarrow$ Non relativistic gas.

A system of N particles $\chi = c \sum |\vec{p}_i| + U(q_i)$

where $U(q_i) = 0$ for $0 \leq q_i \leq L$
 $= \infty$ otherwise

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$V = L^3$

$E = c \sum |\vec{p}_i| \rightarrow$ Ultra relativistic Gas of particles.



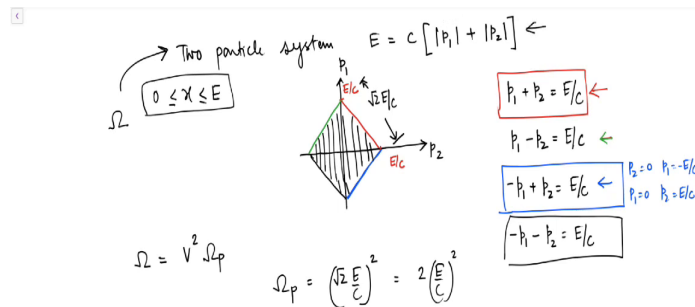
So, in the previous lectures we have used some microcanonical ensemble to look at a paramagnet to a ferromagnet transition. And we have also looked at an ideal gas with the Hamiltonian is sum over i p_i square over twice m .

In the current lecture what we want to now focus on is something similar. A system of N particles, the Hamiltonian of H is given by $C \sum p_i$ plus U of q_i , where U of q_i is equal to 0 , for q_i greater than equal to 0 less than equal to L and is equal to infinity otherwise.

So, essentially what you are looking at is you are looking at a container of volume V is equal to L cube and the particles are contained within this volume. The dispersion relation, so this particular form of the Hamiltonian; so, your total energy is now C times sum over modulus of p_i essentially tells you that you are looking at an ultra relativistic gas of particles.

Here this was a non relativistic gas and we calculated the entropy, the pressure, the equation of state so on and so forth on. Now, we want to look at something like this. Now, it is illustrative and well its instructive to look at two particle system first.

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So, let us look at a two particle system, where the total energy is given by C and C is the velocity of light; so, $\text{mod } p_1$ plus modulus of p_2 . In which case if I draw the phase space, the Hamiltonian does not depend on the coordinates.

And the total energy expression that we have which is essentially the isolating integral in this n particle system also does not depend on the position. So, we only look at p_1, p_2 . Possibilities are p_1 plus p_2 is going to be E over C there is a modulus function. So, that p_1 can take plus and minus values as well.

One has p_1 minus p_2 is equal to E over E by C and then have minus again have minus p_1 plus p_2 is going to be E over C . And finally, I have minus p_1 minus p_2 is going to be E over C . Look at the first equation. So, this equation it clearly tells you that if p_2 is equal to 0, p_1 is E over C and similarly if p_1 is 0, p_2 is going to be E over C .

Therefore this represents the line which is essentially like this. Similarly, for the second one; for the second one I have when p_2 is equal to 0, p_1 is E over C and when p_1 is equal to 0, p_2 is minus E over C . So, I have this line. Well, it does not so, let us make sure that the arms have equal length and then we say that this is going to be E over C . Then again if I look over here, the third equation which is given over here when p_2 is equal to 0, p_1 is minus E over C .

So, p_1 is minus E over C and so, p_2 is equal to 0, p_1 as minus E over C and when p_1 is equal to 0, p_2 as E over C . So, that I have this. And finally, for the last one I have when; I am sorry, one has to be a little bit more careful. So, p_1 is minus E over C which takes you over here and this is the arm that you are looking at and finally, for the last one you will have this arm.

So, the total number of microstates ω for this two particle system when the energy is between the greater than equal to 0 less than equal to E we will just write down over here even though this is a two particle system. And we have learned that we can kind of replace the surface area by the volume only in the thermodynamic limit, but let us just consider this for the time being.

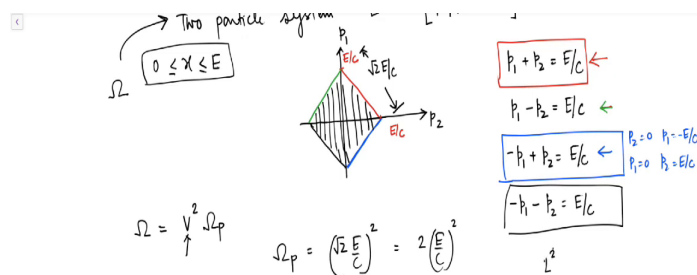
And we want to know the total number of microstates when the energy of the system lies between 0 and E is essentially the area which is contained in this. And that area I know

because this length is a square of length square root 2 E over C, so that the total number of microstates is in the phase space.

The one which is in the phase space is going to be. So, you write as total number of microstates is going to be V square because there are 2 particles and they can access the coordinate space each of them contributing V and then I have omega of p. So, the volume in this momentum space becomes square root 2 E by C whole square which is going to be twice E by C whole square.

Now, be careful that I have not put a vector sign over this momenta. Therefore, I am assuming that this is a one dimensional system and if it is in one dimensional system one has to say that the coordinates this quantity volume is no longer there, it is going to be L square.

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So, you replace the volume.

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$$\Omega = L^2 \Omega_p$$

$$\Omega_p = \left(\sqrt{2} \frac{E}{c}\right)^2 = 2 \left(\frac{E}{c}\right)^2$$

$$= 4 \frac{1}{2} \left(\frac{E}{c}\right)^2$$

Replace the volume by
dimension of your box along
a given direction
 $V \rightarrow L$

Three particle Case: $|p_1| + |p_2| + |p_3| = E/c$

Reduced phase space \rightarrow three dimensional

$$\Omega = L^3 \Omega_p$$



So, you replace the volume by the dimension of your box along a given direction. So, here V therefore, goes to L and you know that for these two particles. So, we will say that this quantity now reduces or goes to L square Ω_p , where Ω_p is given by E by C two times E by C whole square.

So, let us rewrite this in a slightly different way. We will write them as 4 times half E over C whole square, good. Now, we have done it for two particle case. Let us look at it for a three particle case. For a three particle case I have sum over p_i which essentially means $\text{mod } p_1$ plus $\text{mod } p_2$ plus $\text{mod } p_3$ is going to be E over C .

So, that I have a three dimensional momentum. So, the phase space the reduced phase space let us say the reduced phase space is now three dimensional because the Hamiltonian does not depend on the coordinates.

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$\Omega = L^3 \Omega_p$
 $A = \frac{H}{3}$
 $2 \left(\frac{E}{C}\right)^2 \cdot \frac{1}{3} \left(\frac{E}{C}\right) = \frac{2}{3} \left(\frac{E}{C}\right)^3$
 $\Omega_p = 2 \times \frac{2}{3} \left(\frac{E}{C}\right)^3 = \frac{4}{3} \left(\frac{E}{C}\right)^3 = 2 \times \frac{4}{6} \left(\frac{E}{C}\right)^3 = 8 \times \frac{1}{6} \left(\frac{E}{C}\right)^3$
 $\Omega = L^3 \Omega_p = L^3 \left[8 \times \frac{1}{6} \left(\frac{E}{C}\right)^3 \right]$

upper half and lower half has equal volume!!
 $\Omega_p^{N=3}$



So, we write down the total number of microstates now as L cube because there are three particles and each of which can explore a region of size L times omega p. And here this is a three dimensional space. So, let us draw it. So, I have p 1, p 2 and p 3 and I know that in this two dimensional space this is going to be a square of side square root E sorry square root 2 E by C.

This momentum p 3 also has an upper bound and lower bound of plus minus E over C. And therefore, you are effectively looking at a pyramid, a right angled pyramid and then you have

this. Similarly, this joins this. This one comes over here, you have this one and you have this one.

Well, it does not look symmetric in the figure, but you know that both upper half and lower half has equal volumes. Let us take calculate the volume of the upper half and that volume is given by volume of this pyramid. In the upper half is now given by your area times of the base times H divided by 3.

The area we calculated for this rectangular base was $2 E \text{ by } C \text{ whole square times one-third } E \text{ by } C$. So, that this part becomes $2 \text{ by } 3 \text{ times } E \text{ by } C \text{ whole cube}$. But this is only half the volume. So, that the total volume in the momentum space is going to be $2 \text{ into } 2 \text{ by } 3 \text{ } E \text{ by } C \text{ whole cube}$, which is going to be $4 \text{ by } 3 \text{ } E \text{ by } C \text{ whole cube}$. Now, I will multiply this with an additional 2 and bring in a 6 over here.

So, that I have the form $8 \text{ into } E \text{ by } C \text{ whole cube divided by one-sixth sorry multiplied by one-sixth}$. So, for a 2 ok ok [FL]. Let us write down this. So, ω is $L \text{ cube } \omega \text{ p}$ which is $L \text{ cube times } 8 \text{ one-sixth into one-sixth } E \text{ by } C \text{ whole cube}$. Now, the whole game or the whole trick is now to figure out the volume in a hyper dimensional for a hyper dimensional pyramid. That we can do just by looking at these two example. So, when we had $\omega \text{ p}$, N is equal to 2 ok, let us write down over here.

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$$\Omega_p^{N=2} = 2 \left(\frac{E}{C}\right)^2 = 4 \frac{1}{2} \left(\frac{E}{C}\right)^2 = 2^2 \cdot \frac{1}{2!} \left(\frac{E}{C}\right)^2$$

$$\Omega_p^{N=3} = 8 \times \frac{1}{6} \left(\frac{E}{C}\right)^3 = 2^3 \cdot \frac{1}{3!} \left(\frac{E}{C}\right)^3$$

$$\Omega_p^N = 2^N \frac{1}{N!} \left(\frac{E}{C}\right)^N$$

D-dimensional Hyper-pyramid
 $\Omega = \frac{R^D}{D!}$ $\sum x_i = R$
 $(x_i \geq 0)$

The total number of microstates that are contained for $0 \leq x_i \leq E$

$$\Omega = L^N \Omega_p^N = L^N 2^N \frac{1}{N!} \left(\frac{E}{C}\right)^N$$



Omega p N is equal to 2 was 2 half we had sorry we had 2 times E over C whole square which we could have written as 4 times half E by C whole square and that is 2 square times 1 over 2 factorial E by C whole square. When omega p N is equal to 3, we have this as 8 into 1 over 6 E by 6 whole cube which is 2 cube 1 over 3 factorial V by C whole cube.

These two expressions clearly give you the hint what the general expression is going to be. So, I can write down omega p times N is going to be 2 to the power N 1 over N factorial E over C raised to the power N and this is the answer that you are looking for. For a hyper N dimensional ok, we will not say N dimensional.

Let us say for a D dimensional hyper pyramid the volume omega is given by R to the power D divided by D factorial. And the hyper pyramid is defined as sum over x i is equal to R, where x i is greater than 0. If you impose this x i greater than 0 then you have this expression. If you

say that look I do not want to impose then you will come up with this additional factor of 2 and here the additional factor of 2 comes in because the momenta can be either positive or negative.

Therefore, the total number of microstates that are contained for less than equal to E is given by Ω and that answer is going to be L to the power N Ω p N which is going to be L to the power N 2 to the power N 1 over N factorial E by C raised to the power N .

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$$\Omega = \frac{1}{h^N} \frac{L^N}{N!} 2^N \frac{1}{N!} \left(\frac{E}{C}\right)^N$$

$$= \frac{2^N L^N}{N!^2} \left(\frac{E}{hc}\right)^N \leftarrow \begin{matrix} E = h\nu = \frac{hc}{\lambda} \\ \Rightarrow \frac{E}{hc} = \frac{1}{\lambda} \end{matrix}$$

$$\Omega = \frac{2^N}{N!^2} \left(\frac{LE}{hc}\right)^N \rightarrow \text{Dimensionless!!}$$

$$S = k_B \ln \Omega = k_B \ln \left[\frac{2^N}{N!^2} \left(\frac{LE}{hc}\right)^N \right]$$



Now, we still have not taken into account the indistinguishability of the particles. So, that we have Ω L to the power N 2 to the power N divided by N factorial. And there is going to be an h to the power N essentially that non dimensionalizes this because you can see that this is not the thing.

This is a dimension full quantity and I have again a $1/N$ factorial E/hC raised to the power N . So, that I have 2^N by h^N we will take the h inside and we will say that this is L^N over N factorial square E/hC raised to the power N .

So, we have this expression now and if you are doubtful about this then you know that E is going to be $h\nu$, which is going to be hC/λ and this implies that E/hC has a dimension of $1/L$. And exactly you see that this factor which is 2^N divided by N factorial square $L^N E/hC$ raised to the power N is dimensionless as you expect it to be.

So, the entropy, the direct route is now to the entropy which is going to be $k_B \ln$ times ω and therefore, I have $k_B \ln 2^N$ over N factorial square L^N times E/hC raised to the power N .

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$$S = k_B \ln \Omega = k_B \ln \left[\frac{2^N}{N!} \left(\frac{LE}{hC} \right)^N \right]$$

$$= k_B \left[N \ln 2 + N \ln \frac{LE}{hC} - 2 \ln N! \right]$$

$\ln N! = N \ln N - N$

$$S(E, V, N) = k_B \left[N \ln 2 + N \ln \frac{LE}{hC} - 2N \ln N + N \right]$$

$$\left(\frac{\partial S}{\partial V} \right) = \frac{P}{T}$$

$$\left(\frac{\partial S}{\partial L} \right) = k_B \frac{\partial (N \ln L)}{\partial L} = \frac{N k_B}{L}$$

$$\frac{P}{T} = \frac{N k_B}{L}$$

$$P = \beta k_B T \rightarrow \text{Ideal Gas Law!!}$$



Let us open the bracket and split everything up. I have $N \ln 2$ plus $N \ln L E$ over $h C$ minus $2 \ln$ of N factorial, which for a in the thermodynamic limit i can use the Stirling's approximation for this which tells me $\ln N$ factorial is $N \ln N$ minus N .

And one has $k_B N \ln 2$ plus $N \ln L E$ over $h C$ minus $2 N \ln N$ plus N . So, this is the fundamental relation that we have been trying to emphasize in thermodynamics. So, the pressure here is now replaced by $\partial S / \partial L$ that should be the pressure. In the thermodynamic when we did thermodynamics we said that $\partial S / \partial V$ is equal to P / T right.

But here the volume is replaced by the length L and $\partial S / \partial L$ is going to be k_B times $\partial / \partial L$ of $N \ln L$ right. The rest of it does not depend on L . So, it is not very significant for us, the derivative is 0. So, essentially you have $k_B N k_B / L$. So, that the pressure P by T is

going to be $N k_B$ over L and you have the ideal gas law which is P by T is going to be ρ times k_B or pressure is ρ times $k_B T$. The ideal you recovered that very nicely.

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$\frac{P}{T} = \frac{N k_B}{L}$ $P = \rho k_B T \rightarrow \text{Ideal Gas Law!!}$
 $\frac{\partial S}{\partial E} = \frac{1}{T} \Rightarrow \frac{\partial S}{\partial E} = k_B \frac{\partial}{\partial E} \ln E = \frac{N k_B}{E}$
 $\Rightarrow \frac{1}{T} = \frac{N k_B}{E} \Rightarrow E = N k_B T$
 $T dS = dE + P dL$ $C_L = \left. \frac{\partial E}{\partial T} \right|_{L,N} = N k_B$
 $T \frac{\partial S}{\partial T} = \left. \frac{\partial E}{\partial T} \right|_{L,N} + P \left. \frac{\partial L}{\partial T} \right|_{L,N}$
 $C_p = N k_B +$



$\frac{\partial S}{\partial E}$ is going to be $1/T$ right. So, this implies that $\frac{\partial S}{\partial E}$ from this expression is k_B times $\frac{\partial}{\partial E} \ln E$ of $N \ln E$. Rest of it does not matter because they do not depend on the energy and which is $N k_B$ divided by E .

So, that $1/T$ is going to be $N k_B$ over E and this implies E is equal to $N k_B T$. Recall that this was in a one dimension. If you had done it for three dimension, you would have got the result $3 N k_B T$. So, that is precisely the case that you have. This is the dependence of energy of an ultra relativistic gas.

So, for thermodynamics I know that $T dS$ is dE plus $P dL$, one dimensional system, therefore, I have this. So, the two specific heats, this corresponds to the specific heat at constant volume is going to be $\frac{\partial E}{\partial T}$ L N N fixed, which is precisely this relation and is going to be $N k_B$. The specific heat at constant pressure is going to be $T \frac{\partial S}{\partial T}$ P N constant is equal to $\frac{\partial E}{\partial T}$ P N constant plus $P \frac{\partial L}{\partial T}$ P N constant.

Did we do something stupid? No, I think this is correct. This quantity is your C_p and this quantity is your $N k_B$ plus if you look at your equation of state which tells you.

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$$T dS = dE + P dL \quad C_L = \left. \frac{\partial E}{\partial T} \right|_{L,N} = N k_B \leftarrow \text{UR Gas in 1D}$$

$$T \left. \frac{\partial S}{\partial T} \right|_P = \left. \frac{\partial E}{\partial T} \right|_{P,N} + P \left. \frac{\partial L}{\partial T} \right|_{P,N} \quad P L = N k_B T$$

$$\uparrow C_p = N k_B + N k_B \quad P \left. \frac{\partial L}{\partial T} \right|_{P,N} = N k_B$$

$$C_p = 2 N k_B \leftarrow \text{UR Gas in 1D}$$



The equation of state tells you p times L is going to be $N k_B T$ and since I am taking the derivative with P and N held constant. Therefore, $P \frac{\partial L}{\partial T}$ P N constant is going to

be N times k_B , so that this term gives you an additional $N k_B$ and therefore, the specific heat becomes twice $N k_B$.

Please note that this is only for a gas ultra relativistic gas in one dimension. This is also ultra relativistic gas in one dimension if you are changing the dimension. If you are making this to be in three dimension, then this is going to be $3 N k_B$ and this is going to be $6 N k_B$. So, we now want to take up the last example using our microcanonical ensemble and that is of a quantum ideal solid.

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Quantum ideal solid

$E_i = (n_i + \frac{1}{2}) \hbar \omega$

$E = \sum (n_i + \frac{1}{2}) \hbar \omega$

Consider now 2 particles (n_1, n_2) .

$\hbar \omega (n_1 + n_2) + \frac{1}{2} \hbar \omega + \frac{1}{2} \hbar \omega = E$

$n_1 + n_2 = \frac{E - \hbar \omega}{\hbar \omega} = 1$

$E = \hbar \omega$

NPTEL

So, once again the picture is that I have a one dimensional lattice and each of these particles are confined in a harmonic potential which is half $m \omega^2 q^2$. We will consider the one dimensional case so that we can treat each the each of these three

dimensions independently of each other. Therefore, it suffices to calculate for the one dimensional case and generalize it for three dimension.

Now, here the energy levels of each of these particles are discrete and I have the equation ϵ_{n_i} is going to be n_i plus half $\hbar \omega$. So, that the total energy is going to be sum over n_i plus half $\hbar \omega$. Now, let us take specific examples. Consider now 2 particles, which are characterized by n_1 and n_2 .

So, now we have n_1 plus n_2 plus half $\hbar \omega$ plus half $\hbar \omega$ is equal to the total energy times \hbar , this has to be multiplied by ω . And let us say we have E is equal to twice $\hbar \omega$. The total energy I fix it to be twice $\hbar \omega$. Then it follows that n_1 plus n_2 is going to be twice $\hbar \omega$ minus $\hbar \omega$ divided by $\hbar \omega$, which is just going to be 1.

Is this correct? Sorry, this is correct. But, I think we will take this factor later on. We will just say that it is $\hbar \omega$.

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$$E_i = \left(n_i + \frac{1}{2}\right) \hbar \omega \quad \frac{1}{2} m \omega^2 q_i^2$$
$$E = \sum \left(n_i + \frac{1}{2}\right) \hbar \omega$$

Consider now 2 particles (n_1, n_2) :

$$\hbar \omega \left(n_1 + n_2\right) + \frac{1}{2} \hbar \omega + \frac{1}{2} \hbar \omega = E \quad E = \hbar \omega$$
$$n_1 + n_2 = \frac{\hbar \omega - \hbar \omega}{\hbar \omega} = 0$$
$$n_1 = 0, \quad n_2 = 0$$



So, now we fix the total energy E is equal to $\hbar \omega$. This is the total energy of the system. Two particles, two oscillators with the total energy of E equal to $\hbar \omega$ and then you immediately see that $n_1 + n_2$ is going to be $\frac{\hbar \omega - \hbar \omega}{\hbar \omega}$ is equal to 0, which essentially means that n_1 must be 0, n_2 must be 0, no other combinations of n_1 and n_2 are possible.