

Title: Statistical Mechanics (PHYS 602) - Lecture 11

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Abstract:

Bosons and fermions

Second Quantization

- Second Quantization vs Classical

- Quantum Description

- One Mode

Independent Excitations

- Extreme limit for fermions

- Extreme limit for bosons

Waves

- Waves= Special Bosons

- photons in cavity

- waves as independent excitations

Conserved particles

- conserved fermions in a box

- conserved bosons in a box

- bose transition

- dynamics of fermions at low temperatures

- Landau's description

- dynamics of bosons

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In the quantum mechanics of non-interacting particles, each mode is dynamically and statistically independent of the others. That is to say, the Hamiltonian is a sum of terms each referring to a different mode. We have a **discrete infinity** of modes, labelled by the m 's.

A sum over the independent modes in quantum theory can be written as $\sum_{\mathbf{m}}$

Usually, but not always, many terms contribute from such a sum so that it can be written as an integral over wave vectors or momenta in the form

$$\sum_{\mathbf{m}} \rightarrow \left(\frac{L}{2\pi}\right)^3 \int d\mathbf{k} = \left(\frac{L}{2\pi\hbar}\right)^3 \int d\mathbf{p} \quad \text{vi.1}$$

This result is interpreted by saying that the quantum sum over m goes into a sum over phase space in discrete pieces of size h^3 . Of course, there is no h^3 in any sensible formulation of classical mechanics. So something funny will have to be done to patch together classical mechanics and quantum theory.

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A sum over the independent modes in quantum theory can be written as $\sum_{\mathbf{m}}$

Usually, but not always, many terms contribute from such a sum so that it can be written as an integral over wave vectors or momenta in the form

$$\sum_{\mathbf{m}} \rightarrow \left(\frac{L}{2\pi}\right)^3 \int d\mathbf{k} = \left(\frac{L}{2\pi\hbar}\right)^3 \int d\mathbf{p} \quad \text{vi.1}$$

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Usually, but not always, many terms contribute from such a sum so that it can be written as an integral over wave vectors or momenta in the form

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A sum over the independent modes in quantum theory can be written as $\sum_{\mathbf{m}}$

Usually, but not always, many terms contribute from such a sum so that it can be written as an integral over wave vectors or momenta in the form

$$\sum_{\mathbf{m}} \rightarrow \left(\frac{L}{2\pi}\right)^3 \int d\mathbf{k} = \left(\frac{L}{2\pi\hbar}\right)^3 \int d\mathbf{p} \quad \text{vi.1}$$

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$$\sum_{\mathbf{m}} \rightarrow \left(\frac{L}{2\pi}\right)^3 \int d\mathbf{k} = \left(\frac{L}{2\pi\hbar}\right)^3 \int d\mathbf{p} \quad \text{vi.1}$$

This result is interpreted by saying that the quantum sum over m goes into a sum over phase space in discrete pieces of size h^3 . Of course, there is no h^3 in any sensible formulation of classical mechanics. So something funny will have to be done to patch together classical mechanics and quantum theory.

Quantum Description

To describe a degenerate quantum situation, we first specify the modes. We imagine placing everything in a box of side L . One neat formulation has periodic boundary conditions. The different modes of excitation are described by wave functions which are of the form $(1/L)^{3/2} \exp(i\mathbf{k} \cdot \mathbf{r})$. The wave number $\mathbf{k} = (k_x, k_y, k_z)$ must be of the form $(2\pi/L)\mathbf{m} = (2\pi/L)(m_x, m_y, m_z)$ where the m 's are integers. This gives periodic wave functions, and what is more important, a complete set of wave functions. Corresponding to these k 's are momenta, p 's, of the form $\mathbf{p} = \hbar \mathbf{k}$

In the quantum mechanics of non-interacting particles, each mode is dynamically and statistically independent of the others. That is to say, the Hamiltonian is a sum of terms each referring to a different mode. We have a **discrete infinity** of modes, labelled by the m 's.

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Evidence
for Atoms

How
Big Is A
Molecule?

$$k = \frac{2\pi}{L} m$$
$$\sum_m \Delta m \rightarrow \int dm$$

One mode

In the grand canonical formulation, the only difference between bosons and fermions is the possible values of the excitation number of a given type, n_i . For bosons this n can be any non-negative integer 0, 1, 2, ... For fermions the excitation or **mode** can either be empty or occupied, corresponding to $n=0$ or 1. In either the bose or the fermi cases, the probabilities are given by $\rho(n)=(1/\xi) \exp[-\beta(\epsilon-\mu)n]$,

We next look to a single mode of excitation. For the **fermion**, the normalizing factor is $\xi= 1 +\exp[-\beta(\epsilon-\mu)]$

The probability for finding the state full is

$$\langle n \rangle = 1 / \{1 +\exp[\beta(\epsilon-\mu)]\} \quad \text{vi.2a}$$

The probability for finding the state empty is

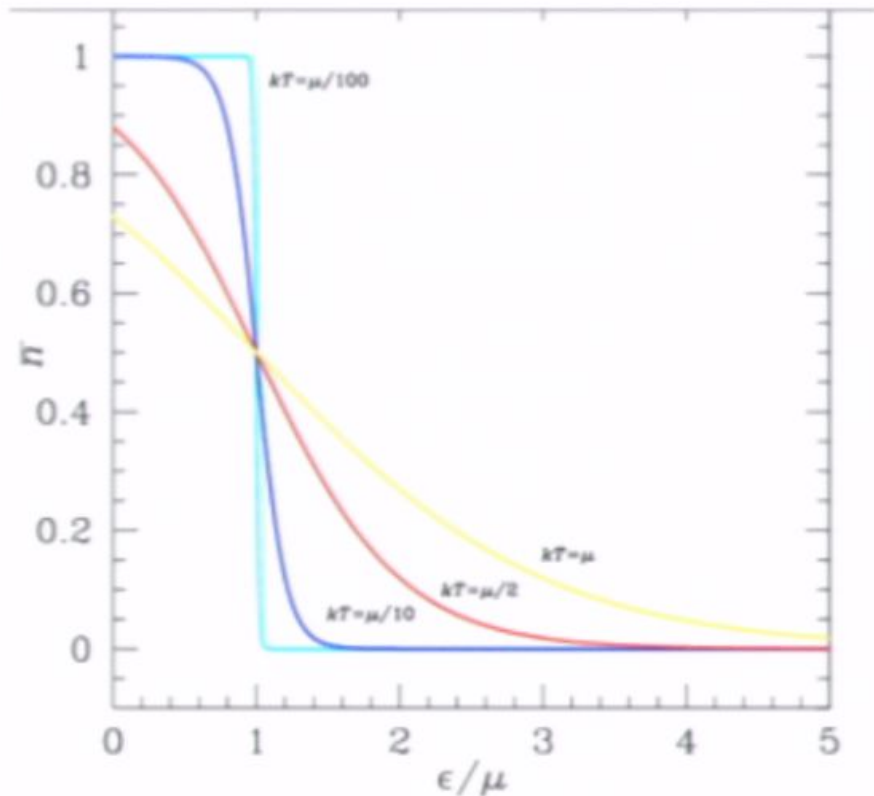
$$1-\langle n \rangle = 1 / \{1 +\exp[-\beta(\epsilon-\mu)]\} \quad \text{vi.2b}$$



Extreme Limits for fermions

The extreme quantum limit is the one with large values of $\beta \mu = \mu/(kT)$. In that limit the mode is always completely full (empty) depending on whether $(\epsilon - \mu)$ is negative (positive).

The extreme classical limit is the one with large values of $-\beta \mu$. In that limit, in equilibrium, all modes have a very low probability of being occupied and $\langle n \rangle \approx \exp[-\beta(\epsilon - \mu)]$



This picture gives plots of $\langle n \rangle$ versus ϵ/μ for various values of $1/(\beta \mu)$. The large numbers indicate highly degenerate situations, while the smaller ones are closer to the classical limit.

Grains of
Pollen to
Evidence
for Atom

How
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$$k = \frac{2\pi}{\lambda} m$$

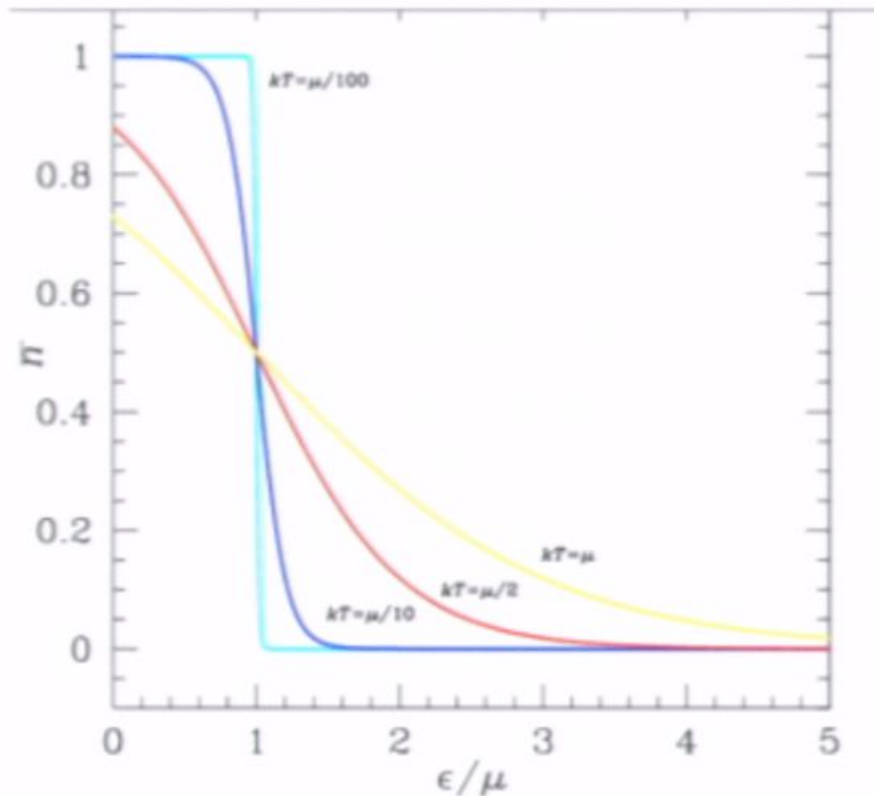
$$\sum_m \Delta m \rightarrow \int dm$$

$$\beta \left(\epsilon - \mu - \frac{1}{2} m v^2 \right)$$

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$$\langle n \rangle \approx$$

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For the boson

the equilibrium probability distribution for occupation of the single mode is $\rho(n) = (1/\xi) \exp[-\beta(\epsilon - \mu)n]$. All integer values of n between zero and infinity are permitted.

The normalizing factor is

$$\xi = 1 + \exp[-\beta(\epsilon - \mu)] + \exp[-2\beta(\epsilon - \mu)] + \exp[-3\beta(\epsilon - \mu)] + \dots$$

$$\xi = 1 / \{1 - \exp[-\beta(\epsilon - \mu)]\}$$

Note that $\epsilon - \mu$ must be positive.

The average occupation is $\langle n \rangle = 1 / \{\exp[\beta(\epsilon - \mu)] - 1\}$ vi.3 **show this**

An extreme quantum limit is the one with very small positive values of $\beta(\epsilon - \mu)$. In that limit, the mode can have lots and lots of quanta in it. You can even have **macroscopic occupation of a single mode**, in which a finite fraction of the entire number of particles is in a single mode. This is also called **Bose-Einstein** condensation after the discoverers of this effect.

The extreme classical limit is once more a very large value of $-\beta\mu$ and a small average occupation of the state. Once more $\langle n \rangle \approx \exp[-\beta(\epsilon - \mu)]$ in this limit.



Satyendra Nath Bose

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Independent Excitations: waves

One example of a boson excitation is provided by a set of waves. There are two major examples: light waves and sound waves. In these two cases, the quanta are called respectively photons and phonons. In the simplest situation, the Hamiltonian for the system is a sum over terms corresponding to the different excitations in the system

$$\mathcal{H} = \sum_j \epsilon_j n_j \quad \text{vi.4}$$

and the statistical mechanics is given by the usual formula

$$\rho\{n\} = (1/\Xi) \exp(-\beta \mathcal{H}\{n\})$$

where the normalizer, Ξ , is called the grand partition function.

Here, ϵ_j is the energy of a single excitation of type j and n_j is the number of excitations of that type. These quanta have the property that they are not conserved. When the basic objects under consideration are conserved quantities, e.g. atoms or molecules, and they don't interact, the Hamiltonian is of exactly the same form, but it is convenient to use a statistical theory in which we allow the total number of particles to vary, and use a probability function of the form

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$$\mathcal{H} = \sum_j \epsilon_j n_j \quad \text{vi.4}$$

and the statistical mechanics is given by the usual formula

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where the normalizer, Ξ , is called the grand partition function.

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Waves=Special bosons

$\epsilon = \hbar\omega$, so in the classical limit the energy of a photon goes to zero.

the probability distribution for the single mode is

$$\rho(n) = (1/\xi) \exp[-\beta \epsilon n]$$

The normalizing factor is

$\xi = 1 + \exp[-\beta \epsilon] + \exp[-2\beta \epsilon] + \exp[-3\beta \epsilon] + \dots$ so that

$$\xi = \frac{1}{1 - \exp[-\beta \epsilon]}$$

Note that ϵ must be positive or zero. The average energy in the mode is

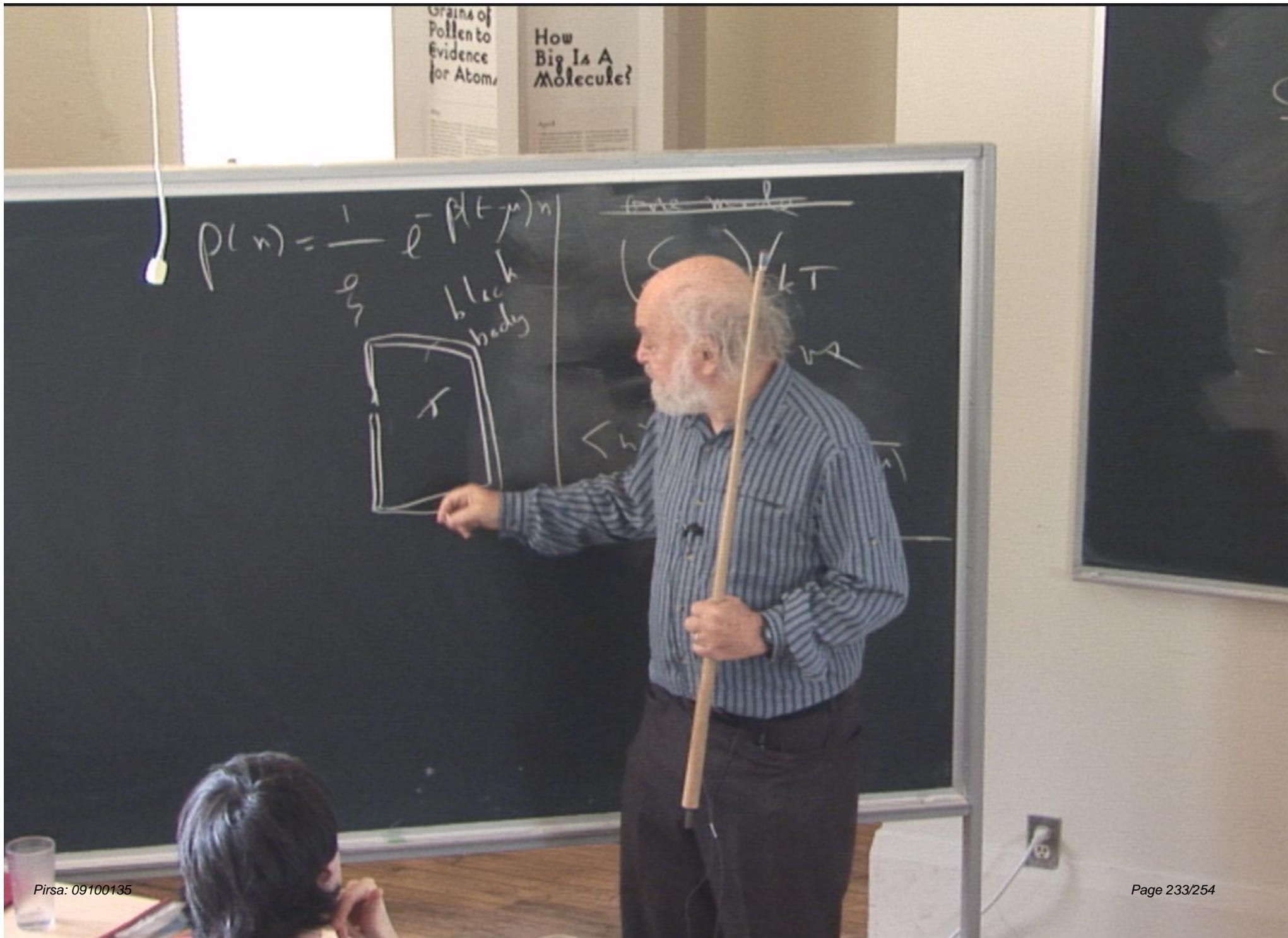
$$\langle n \rangle \epsilon = \epsilon / \{ \exp[\beta \epsilon] - 1 \} = \hbar\omega / \{ \exp[\beta \hbar\omega] - 1 \}$$

Classical limit = high temperature $\langle n \rangle \epsilon = 1 / \beta = kT$

Therefore classical physics gives kT per mode. A cavity has an infinite number of electromagnetic modes. Therefore, a cavity has infinite energy?!?

In quantum theory high frequency modes are cut off because they must have small average occupations numbers, $\langle n \rangle$. Therefore the classical result of kT per mode is simply wrong. So there is no infinity.

In this way, Planck helped us get the right answer by introducing photons and starting off the talk about occupation numbers!



Grains of Pollen to Evidence for Atoms
How Big Is A Molecule?

$$p(n) = \frac{1}{\mathcal{Z}} e^{-\beta(E_n - \mu)n}$$

black body



$(\dots) \sqrt{kT}$
 v_r

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~~one mode~~

$$(E - \mu)/kT$$

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black
body

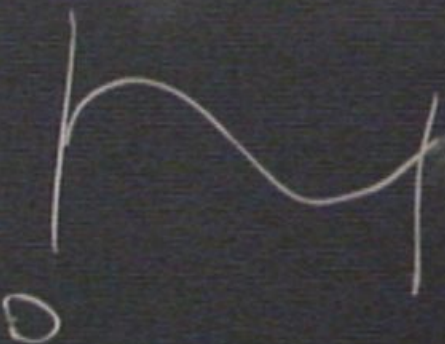


~~one more~~

$$(\Sigma - \mu)/kT$$

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$$(\epsilon - \mu)/kT$$

$\langle n \rangle$

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photons in Cubic Cavity

$\mathbf{k}=(k_x,k_y,k_z)=2\pi(m_x,m_y,m_z)/L$ where the m 's are integers describing the cavity's modes
Here $\omega=ck$ (There are two modes for each frequency)

$$\mathcal{H} = \sum_{\mathbf{m},\sigma} n_{\mathbf{m},\sigma} \hbar ck(\mathbf{m})$$

We can then find the average energy in the form

$$\langle \mathcal{H} \rangle = 2 \sum_{\mathbf{m}} n_{\mathbf{m},\sigma} \hbar ck(\mathbf{m}) \frac{1}{\exp(\beta \hbar ck(\mathbf{m})) - 1}$$

If the box is big enough, the sum over \mathbf{m} can be converted into an integral over \mathbf{k} .

$$\langle \mathcal{H} \rangle = 2 \left(\frac{L}{2\pi} \right)^3 \int d^3k \hbar ck \frac{1}{\exp(\beta \hbar ck) - 1}$$

The integration variable can then be made dimensionless

$$\langle \mathcal{H} \rangle = \frac{2}{\beta} \left(\frac{L}{2\pi \hbar ck} \right)^3 \int d^3q q \frac{1}{\exp(q) - 1}$$

and the integral rewritten in a form which converges nicely at zero and infinity.

$$\langle \mathcal{H} \rangle = 2(kT)^4 \left(\frac{L}{2\pi \hbar ck} \right)^3 \int_0^\infty dq 4\pi q^3 \frac{1}{\exp(q) - 1}$$

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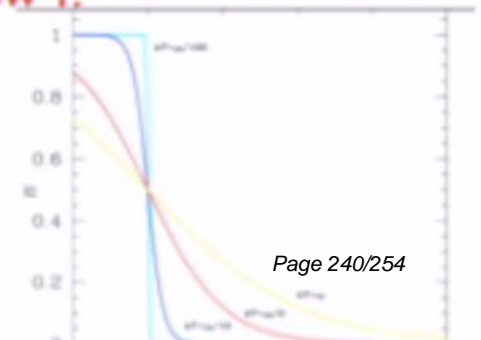
Paul Dirac has a beautiful quantum mechanics book which I enjoyed reading when I was a grad student.

Conserved Fermions in Box

In a metal electrons act as independent quasiparticles with energy and momentum relation ϵ_p . For modes with energy near the value of the chemical potential, these modes behave very much like non-interacting particles with a changed energy-momentum relation. For example they move with a velocity $\mathbf{v} = \nabla_p \epsilon_p$. Only the electrons with energies close to the chemical potential, called in this context the Fermi energy, play an important role in moving heat and particles through the system. The electrons near the Fermi energy are said to be close to the top of the Fermi sea. For lesser energies, within that sea, the electrons are mostly frozen into their momentum states and cannot do much.

For some materials, like Aluminum, $\epsilon_p \approx p^2/(2m)$. For these the Fermi sea forms a ball with radius p_F .

Calculate the $T=0$ energy density, particle density, and pressure of these electrons in terms of p_F . You may use the free particle energy-momentum relation. Harder: Calculate the entropy density as a function of T at low T .



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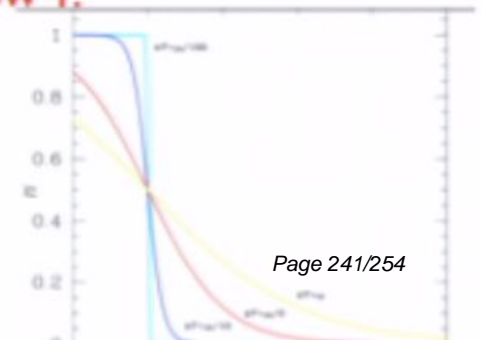
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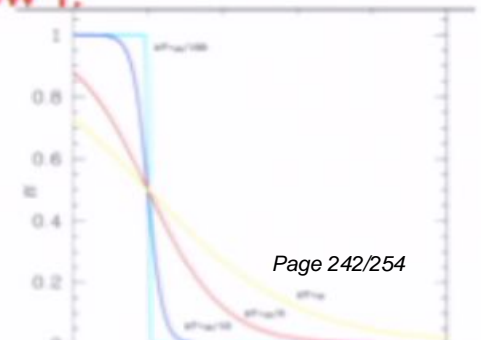
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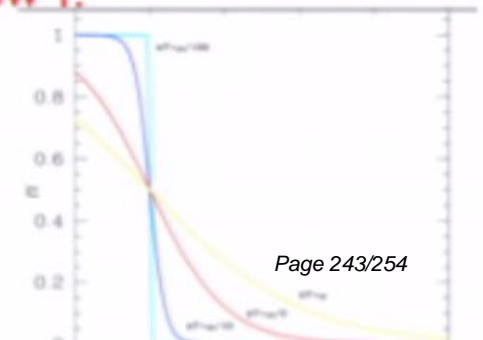
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Conserved Fermions in Box

In a metal electrons act as independent quasiparticles with energy and momentum relation ϵ_p . For modes with energy near the value of the chemical potential, these modes behave very much like non-interacting particles with a changed energy-momentum relation. For example they move with a velocity $\mathbf{v} = \nabla_p \epsilon_p$. Only the electrons with energies close to the chemical potential, called in this context the Fermi energy, play an important role in moving heat and particles through the system. The electrons near the Fermi energy are said to be close to the top of the Fermi sea. For lesser energies, within that sea, the electrons are mostly frozen into their momentum states and cannot do much.

For some materials, like Aluminum, $\epsilon_p \approx p^2/(2m)$. For these the Fermi sea forms a ball with radius p_F .

Calculate the $T=0$ energy density, particle density, and pressure of these electrons in terms of p_F . You may use the free particle energy-momentum relation. Harder: Calculate the entropy density as a function of T at low T .



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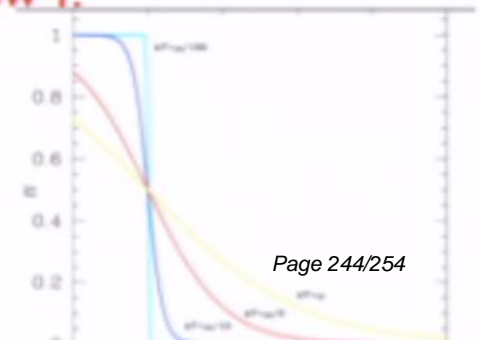
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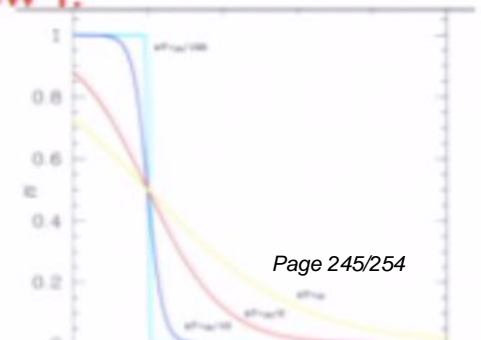
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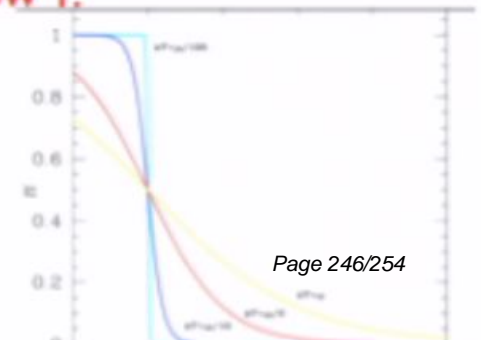
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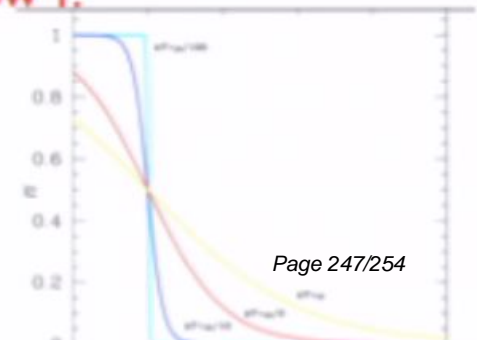
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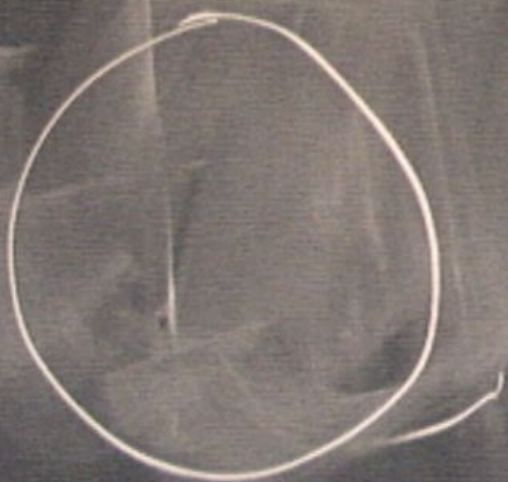


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$n) = \dots$
 q
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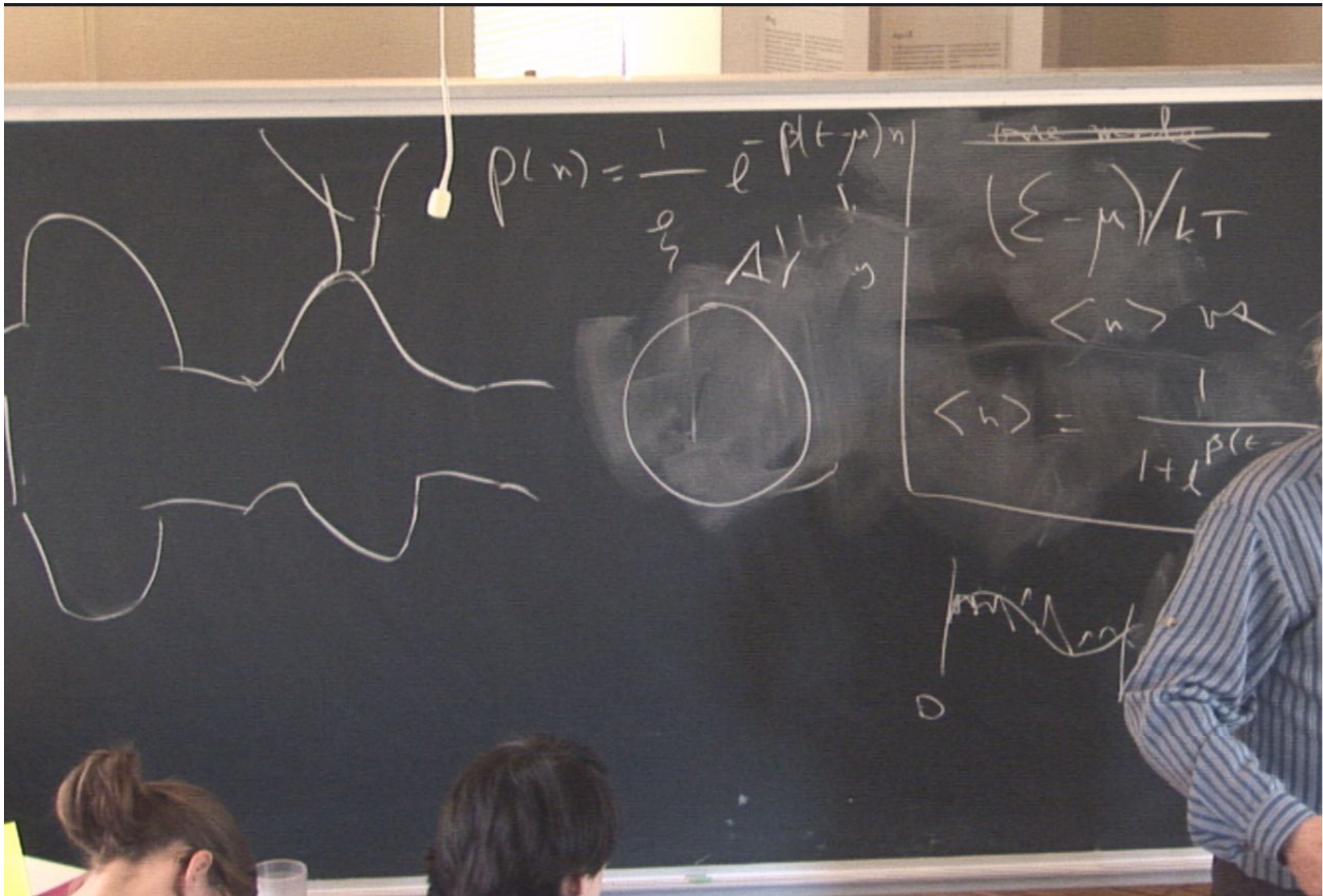


$$(\epsilon - \mu) / kT$$

$$\langle n \rangle$$

$$\langle n \rangle = \frac{1}{1 + e^{\beta(\epsilon - \mu)}}$$





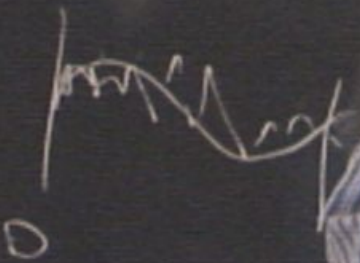
$$p(n) = \frac{1}{\Omega} e^{-\beta(\epsilon - \mu)n}$$

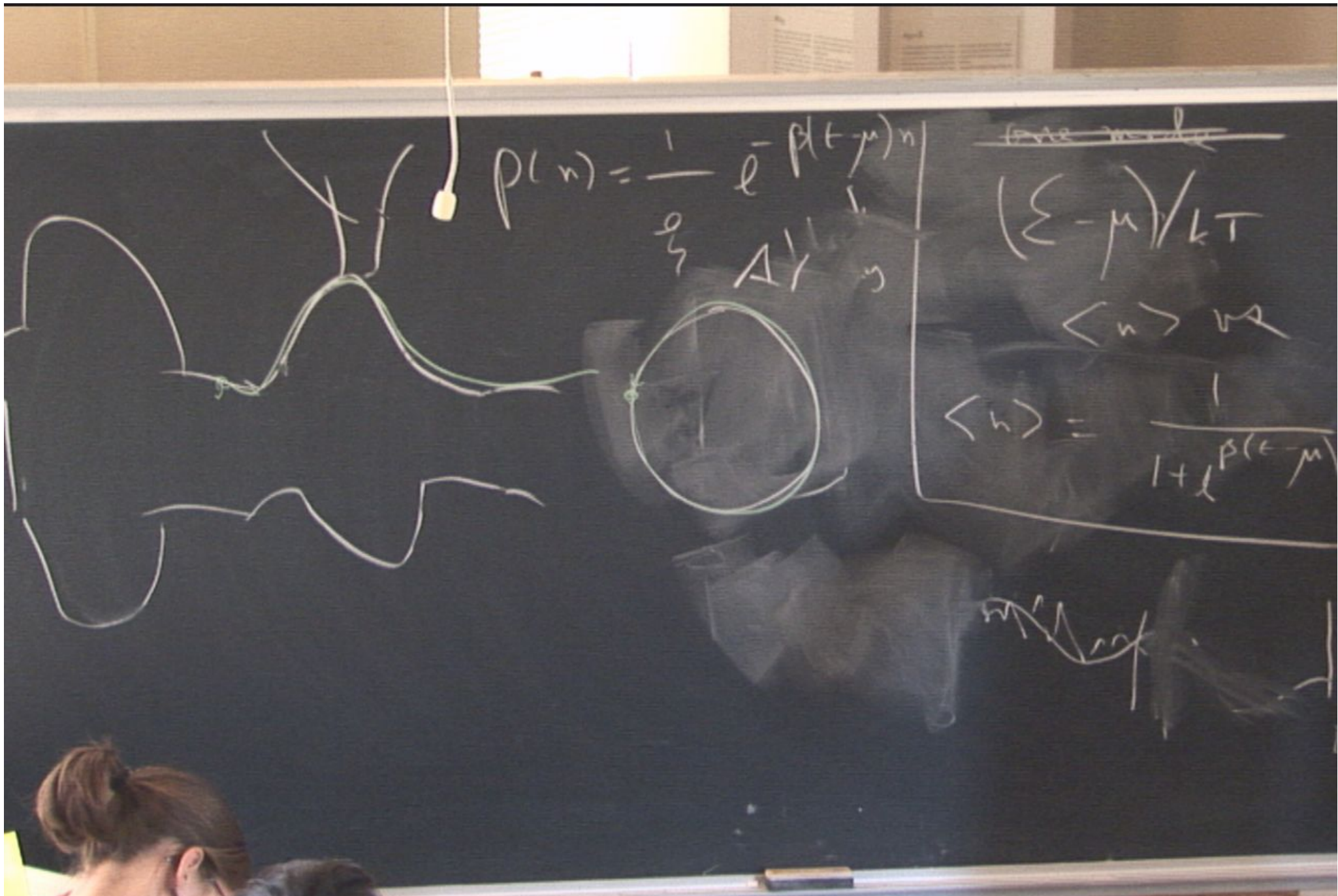
~~free energy~~

$$(\Sigma - \mu)/kT$$

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$$p(n) = \frac{1}{q} e^{-\beta(\epsilon - \mu)n}$$

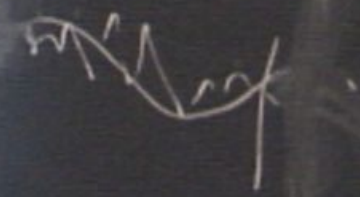
q Δ

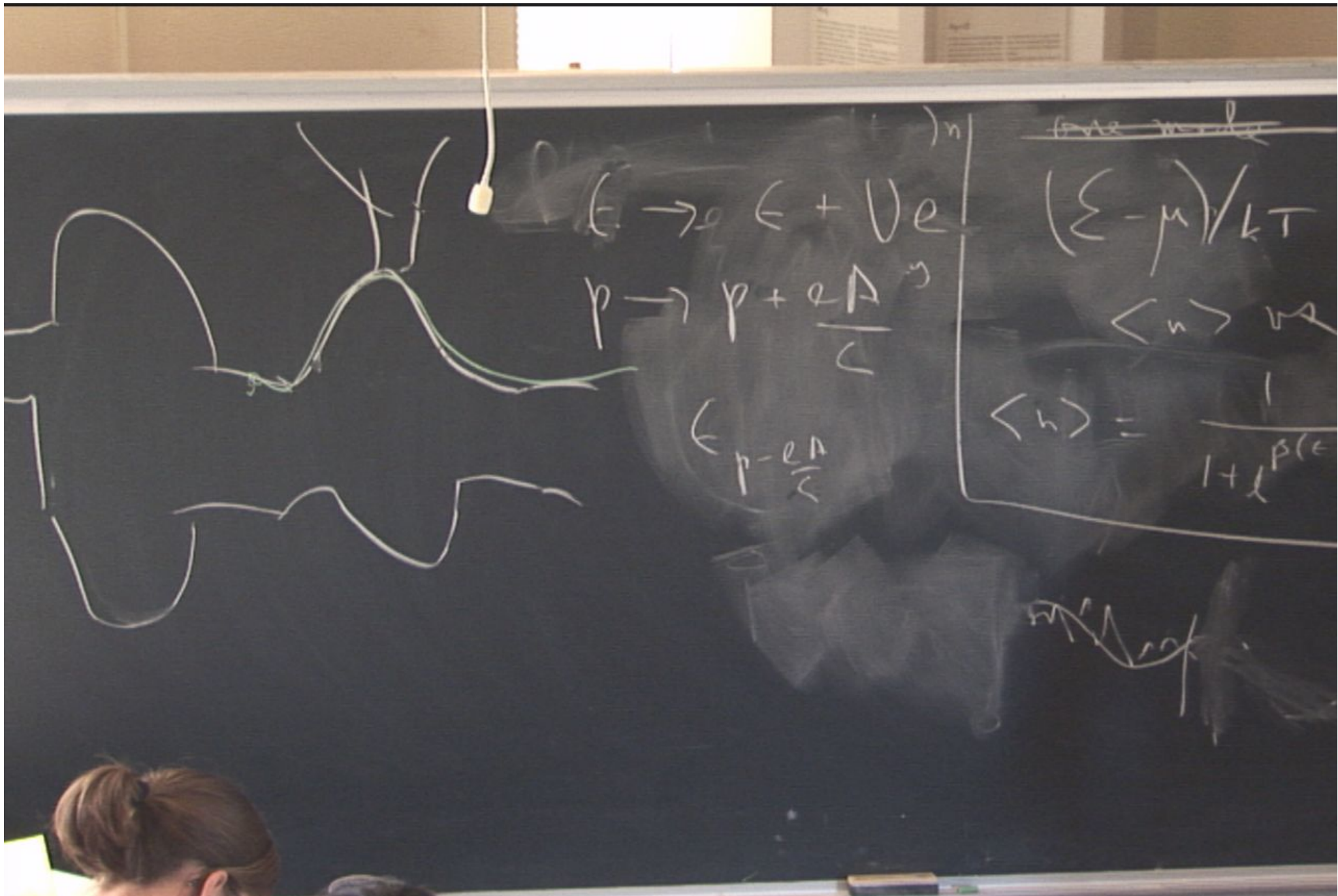
~~one more~~

$$(\Sigma - \mu)/kT$$

$$\langle n \rangle \text{ var}$$

$$\langle n \rangle = \frac{1}{1 + e^{\beta(\epsilon - \mu)}}$$





Conserved Bosons in Box

At low temperatures fluid Helium⁴, that is bosonic helium, undergoes a phase transition into a superfluid state in which it can move without viscosity. This is believed to arise because a finite fraction of the entire number of atoms falls into a single quantum mode, described by a single wave function. The basic theory of how this occurs is due to Nikolay Nikolaevich Bogolyubov.



Nikolay Nikolaevich Bogolyubov

The Einstein-Bose theory of a phase transition in a non-interaction Bose liquid is a pale reflection of the real superfluid transition. However, it is quite interesting both in its own right and also because the recent development of low temperature-low density Bose atomic or molecular gases may make it possible to observe this weak-interaction-effect.

I shall outline the three dimensional theory. The theory in two dimensions is more complex.

Bose Transition

$$n = \text{number of particles per unit volume} = \frac{1}{L^3} \sum_{\mathbf{m}} \frac{1}{1 + \exp\{\beta[\varepsilon(\mathbf{m}) - \mu]\}}$$

Here the sum is over a vector of integers of length three, and the energy is $\varepsilon(\mathbf{m}) = \mathbf{m}^2 \hbar^2 / (2ML^2)$, M being the mass of the particle. For a sufficiently large box, there are two qualitatively different contributions to the sum. The term in which $\mathbf{m} = \mathbf{0}$ can be arbitrarily large because μ can be arbitrarily small. The remaining terms contribute to an integral which remains bounded as μ goes to zero. The result is

$$n = \frac{1}{-L^3 \beta \mu} + \int \frac{d\mathbf{p}}{h^3} \frac{1}{1 + \exp[\beta \frac{p^2}{2M} - \beta \mu]}$$

The integration has a result that goes to zero as T^3 as the temperature goes to zero. If this system is to maintain a non-zero density as T goes to zero, which we believe it can, it can do so by having the first term on the right become large enough so that a finite proportion of the entire number of particles in the system will fall into the lowest mode. This is believed to be the basic source of superfluidity.

Dynamics of fermions at low temperature

Landau described fermions at low temperature by saying that they had a free energy which depended upon, $f(\mathbf{p}, \mathbf{r}, t)$ the occupations of the fermion modes with momentum in the neighborhood of \mathbf{p} and position in the neighborhood of \mathbf{r} at time t . As the occupations changed the free energy would change by

$$\delta F = \int \frac{d\mathbf{p} d\mathbf{r}}{h^3} \epsilon(\mathbf{p}, \mathbf{r}, t) \delta f(\mathbf{p}, \mathbf{r}, t)$$

Then, using the usual Poisson bracket dynamics the distribution function would obey, as in equation v.13.

$$\partial_t f(\mathbf{p}, \mathbf{r}, t) + (\nabla_{\mathbf{p}} \epsilon(\mathbf{p}, \mathbf{r}, t)) \cdot \nabla_{\mathbf{r}} f(\mathbf{p}, \mathbf{r}, t) - (\nabla_{\mathbf{r}} \epsilon(\mathbf{p}, \mathbf{r}, t)) \cdot \nabla_{\mathbf{p}} f(\mathbf{p}, \mathbf{r}, t) \\ = \text{collision term}$$

The collision term will be the same as in the classical Boltzmann equation with one important difference: Since fermions cannot enter an occupied state, the probabilities of entering a final state will be multiplied by a factor of $(1-f)$. Thus, Landau proposed a "Boltzmann equation" for degenerate fermions of the form below, **with the new terms in red**

$$[\partial_t + (\nabla_{\mathbf{p}} \epsilon) \cdot \nabla_{\mathbf{r}} - (\nabla_{\mathbf{r}} \epsilon) \cdot \nabla_{\mathbf{p}}] f(\mathbf{p}) =$$

$$- \iiint d\mathbf{q} d\mathbf{p}' d\mathbf{q}' \delta(\mathbf{p} + \mathbf{q} - \mathbf{p}' - \mathbf{q}') \delta(\epsilon(\mathbf{p}) + \epsilon(\mathbf{q}) - \epsilon(\mathbf{p}') - \epsilon(\mathbf{q}'))$$