PHY 341/641 Thermodynamics and Statistical Mechanics
MWF: Online at 12 PM & FTF at 2 PM

Record!!!

Discussion for Lecture 27:

Quantum effects in statistical mechanics

Reading: Chapter 7 (mostly 7.3)

1. **Recap of statistical mechanics for photons (blackbody radiation)**
2. **Statistical mechanics of Bose particles**
3. **Statistical mechanics of Fermi particles**
4. **Examples**

21	Mon: 03/22/2021	Chap. 6.1 & 6.5	Microcanonical and canonical ensembles		
22	Wed: 03/24/2021	Chap. 6.1-6.2	Canonical distributions	#18	03/26/2021
23	Fri: 03/26/2021	Chap. 6.1-6.7	Canonical distributions	6.49	03/29/2021
24	Mon: 03/29/2021	Chap. 6.1-6.7	Canonical distributions	#20	03/31/2021
25	Wed: 03/31/2021	App. A & Chap. 7.1	Quantum mechanical effects	#21	04/02/2021
26	Fri: 04/02/2021	Chap. 7.1-7.2	Quantum mechanical effects		
27	Mon: 04/05/2021	Chap. 7.3	Bose and Fermi statistics	#22	04/09/2021
	Wed: 04/07/2021	No class	*Holiday*		
28	Fri: 04/09/2021	Chap. 7.4	Bose and Fermi statistics		

PHY 341/641 -- Assignment #22

April 5, 2021

Continue reading Chapter 7 in **Schroeder** .

This is an exercise illustrating the use of the Dirac delta function $\delta(x)$. Assume that all integrals are performed over the range of $-\infty < x < \infty$ and that $f(x)$ has values and zeros within the same range. "a" and "b" denote positive real numbers. valuate the following integrals performed over the full range of x having the form $\int dx\, G(x)\, \delta(b-f(x))$ where $G(x)$ and $f(x)$ are specified below:

1. $G(x)=x$ and $f(x)=ax$
2. $G(x)=x^2$ and $f(x)=ax$
3. $G(x)=x$ and $f(x)=ax^2$
4. $G(x)=x^2$ and $f(x)=ax^2$

PHYSICS COLLOQUIUM

4 PM

THURSDAY

APRIL 8, 2021

"Can Next-Generation 6G Mobile Communications Above 100 GHz Find a Way to Coexist with Passive Satellites Used for Weather and Environmental Sensing?"

Radio frequencies above 100 GHz presently have little actual use except for passive systems used for radio astronomy and for satellite-based sensing of weather data and pollution monitoring. But new technology and the growing demands for terrestrial telecom such as smart phones has resulted in growing needs for capacity in 5G and 6G systems. Some of this capacity is expected to be above 100 GHz for policy decisions in the 1980s and 90s set aside many blocks of spectrum for purely passive systems to a much greater degree than in lower frequencies. A major challenge is thus how can we shoehorn both uses into the same spectrum. Fortunately the quirky nature of radio propagation above 100 GHz offers some possible paths as does the small wavelengths here that permit novel antenna designs. The talk will review possible building blocks of such a solution and technical issues that need to be resolved.

Dr. Michael J. Marcus
Marcus Spectrum Solutions, LLC
Washington, DC

4:00 pm
Via Video Conference

Review: Blackbody radiation. Photons are spin 1 particles which obey Bose statistics.

We learned that for Bose statistics, any number of particles can occupy each state. For photons the total number of particles is not fixed. For a state of energy $\epsilon_s \geq 0$, in thermal equilibrium at temperature T, the partial single particle partition function is given by $(\beta = 1/kT)$

$$Z_1(\epsilon_s, T) = \sum_{n=0}^{\infty} e^{-n\beta\epsilon_s} = 1 + e^{-\beta\epsilon_s} + e^{-2\beta\epsilon_s} + e^{-3\beta\epsilon_s} + ... = \frac{1}{1 - e^{-\beta\epsilon_s}}$$

The partition function of the system combines the independent contributions from all of the states s

$$Z_{Bose}(T) = \prod_s Z_1(\epsilon_s, T) \qquad \Rightarrow \ln\left(Z_{Bose}(T)\right) = -\sum_s \ln\left(1 - e^{-\beta\epsilon_s}\right)$$

Helmholtz free energy:

$$F_{Bose}(T) = -kT \ln Z_{Bose}(T) = kT \sum_s \ln\left(1 - e^{-\beta\epsilon_s}\right)$$

In practice, the state energies ϵ_s form a continuum

$$\sum_s \to \int d\epsilon \; g(\epsilon) \qquad \text{where } g(\epsilon) \text{ denotes the density of states}$$

$$g(\epsilon) = \frac{8\pi V \epsilon^2}{h^3 c^3}$$

$$F(T) = kT \frac{8\pi V}{h^3 c^3} \int_0^\infty d\epsilon \; \epsilon^2 \ln\left(1 - e^{-\beta\epsilon}\right) = \frac{8\pi V (kT)^4}{h^3 c^3} \int_0^\infty dx \, x^2 \ln\left(1 - e^{-x}\right)$$

$$= -\frac{8\pi V (kT)^4}{h^3 c^3} \frac{\pi^4}{45} = U - TS$$

Bose statistics of blackbody radiation -- continued

$$F(T) = -\frac{8\pi V(kT)^4}{h^3c^3}\frac{\pi^4}{45} = U - TS$$

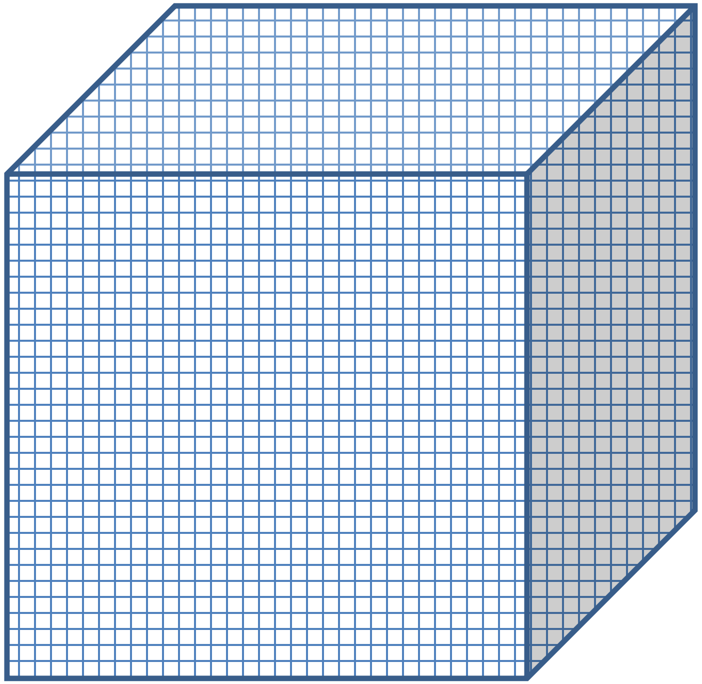
Further relationships --

$$S = -\left(\frac{\partial F}{\partial T}\right)_V = \frac{32\pi V k^4 T^3}{h^3 c^3}\frac{\pi^4}{45}$$

$$U = F + ST = \frac{8\pi^5 V k^4 T^4}{15 h^3 c^3}$$

Comment on density of states

Electromagnetic modes within volume V=L^3



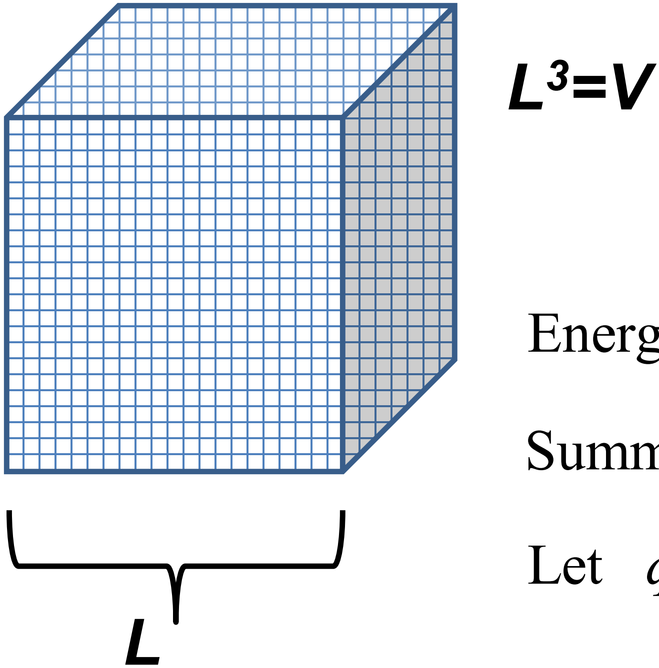
$$\epsilon = \frac{hc}{L}\sqrt{n_x^2 + n_y^2 + n_z^2}$$

for integers n_x, n_y, n_z

In the limit that $L \rightarrow \infty$,

ϵ becomes continuous.

Note that g(ϵ) accounts for two polarizations of photons.



Energy for photon: $\epsilon = \frac{hc}{L}\sqrt{n_x^2 + n_y^2 + n_z^2}$

Summing over all modes $(n_x . n_y , n_z)$ in continuum limit:

Let $q \equiv \sqrt{n_x^2 + n_y^2 + n_z^2}$ $\quad \int dn_x \int dn_y \int dn_z = 4\pi \int q^2 dq$

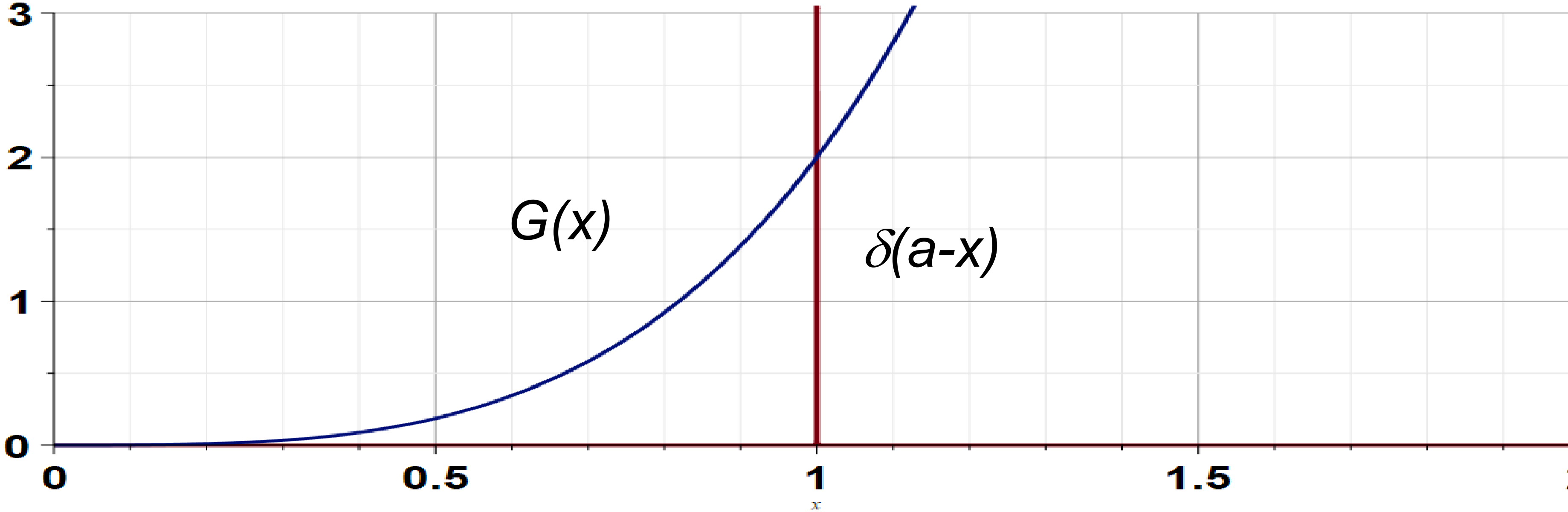
$$g(\epsilon) = 2\; 4\pi \int q^2 dq \;\delta\left(\epsilon - \frac{hcq}{L}\right)$$

2 polarizations

Note that $\int dx\, f(x)\; \delta(a - x) = f(a)$

Let $x = \frac{hcq}{L}$ $\quad g(\epsilon) = 2\; 4\pi \left(\frac{L}{hc}\right)^3 \int x^2 dx\; \delta(\epsilon - x)$

$$g(\epsilon) = \frac{8\pi V \epsilon^2}{h^3 c^3} \qquad V \equiv L^3$$



Comment on integrals over the Dirac delta function

Note that for a smooth function $G(x)$: $\int dx\ G(x)\ \delta(a-x) = G(a)$

What about a more complicated integral such as

$$\int dx\ G(x)\ \delta(a-bx^5) = ?$$

Hint: Make a Taylor expansion of the argument of the delta function

about $a-bx^5=0$ $\quad a-bx^5 \approx 0 + \left(x-\left(\frac{a}{b}\right)^{1/5}\right) 5b\left(\frac{a}{b}\right)^{4/5} + \ldots$

The case of photon statistical analysis was simplified by the fact that any number of photons can contribute to the system. However, for particle systems, the number of particles need part of the analysis.

Another way of evaluating a partition function for a Bose system:

$$Z(T) = \sum_{n_1 n_2 n_3 \ldots\ldots} \exp(-\beta(n_1\epsilon_1 + n_2\epsilon_2 + n_3\epsilon_{3\ldots\ldots}))$$

Here we sum over all occupation numbers n_s and energies ϵ_s.

For N particles, the occupation numbers have the condition

$N = \sum_s n_s$ so that we can calculate the partition for

N particles -- $Z(T,N)$. This is generally difficult, since

$Z(T,N)$ is a rapidly varying function of N.

Note that the following discussion follows the textbook F. Reif, "Fundamentals of Statistical and Thermal Physics" (1965)

Clever trick: Assume that $Z(T,N)$ has an exponential variation with N so that by choosing a parameter α, we can form the so-called "grand partition function"

$$Z_{Grand}(T) \equiv \sum_{N'} Z(T,N')\, e^{-\alpha N'} \approx Z(T,N)\, e^{-\alpha N} w$$

where w is a numerically small value related to the width the peak of the function at the maximum value of N. Taking the log --

$$\ln\left(Z_{Grand}(T)\right) \approx \ln\left(Z(T,N)\right) - \alpha N$$

Why is this a good idea?

Evaluating the Grand Partition Function for the Bose system

$$Z_{Grand}(T) \equiv \sum_{N'} Z(T,N')\, e^{-\alpha N'}$$

$$= \left(\sum_{n_1=0}^{\infty} e^{-(\alpha+\beta\epsilon_1)n_1} \right) \left(\sum_{n_2=0}^{\infty} e^{-(\alpha+\beta\epsilon_2)n_2} \right) \left(\sum_{n_3=0}^{\infty} e^{-(\alpha+\beta\epsilon_3)n_3} \right) \cdots\cdots$$

$$= \left(\frac{1}{1-e^{-(\alpha+\beta\epsilon_1)}} \right) \left(\frac{1}{1-e^{-(\alpha+\beta\epsilon_2)}} \right) \left(\frac{1}{1-e^{-(\alpha+\beta\epsilon_3)}} \right) \cdots\cdots\cdots$$

$$\Rightarrow \ln\left(Z_{Grand}(T)\right) = -\sum_{s} \ln\left(1-e^{-(\alpha+\beta\epsilon_s)}\right) \approx \ln\left(Z(T,N)\right) - \alpha N$$

Obviously, α must depend upon *N*

$$Z_{Grand}(T) \equiv \sum_{N'} Z(T,N')\, e^{-\alpha N'}$$

Peak of $Z(T,N')\, e^{-\alpha N'}$:

$$\left.\frac{\partial\left(\ln\left(Z(T,N')\right)-\alpha N'\right)}{\partial N'}\right|_{N'=N} = 0$$

$$\Rightarrow \frac{\partial \ln\left(Z(T,N)\right)}{\partial N} - \alpha = 0$$

Recall that $\ln\left(Z(T,N)\right) \approx \ln\left(Z_{Grand}(T)\right) + \alpha N$

Also recall that α is a function of N

$$\frac{\partial \ln\left(Z(T,N)\right)}{\partial N} = \frac{\partial \ln\left(Z_{Grand}(T)\right)}{\partial \alpha}\frac{\partial \alpha}{\partial N} + \frac{\partial \alpha}{\partial N} N + \alpha$$

$$\Rightarrow \frac{\partial \ln\left(Z_{Grand}(T)\right)}{\partial \alpha} = N$$

➔Recipe for determining α

$$\frac{\partial \ln\left(Z_{Grand}(T)\right)}{\partial \alpha} = N$$

For the case of Bose particles:

$$\ln\left(Z_{Grand}(T)\right) = -\sum_s \ln\left(1 - e^{-(\alpha+\beta\epsilon_s)}\right)$$

$$\frac{\partial \ln\left(Z_{Grand}(T)\right)}{\partial \alpha} = \sum_s \frac{e^{-(\alpha+\beta\epsilon_s)}}{1 - e^{-(\alpha+\beta\epsilon_s)}} = \sum_s \frac{1}{e^{(\alpha+\beta\epsilon_s)} - 1} = N$$

Relationship of α with quantities we know.

Recall that the chemical potential is given by

$$\mu = \frac{\partial F}{\partial N} = -kT \frac{\partial \ln\left(Z(T,N)\right)}{\partial N} = -kT\alpha$$

$$\Rightarrow \alpha = -\beta\mu$$

$$\Rightarrow \sum_s \frac{1}{e^{\beta(\epsilon_s - \mu)} - 1} = N$$

Summary of results for Bose particles

$$\ln\left(Z_{GrandBose}(T,\mu)\right) = -\sum_s \ln\left(1 - e^{-\beta(\epsilon_s - \mu)}\right)$$

$$\sum_s \frac{1}{e^{\beta(\epsilon_s-\mu)} - 1} = N$$

When the energy levels of our system are continuous, the summation over states *s* will change into the integral of energies ε with the density of states function g(ε).

Statistical mechanics of Fermi particles, analyzed using a similar approach --

Introducing the chemical potential to evaluate the Grand Partition Function for Fermi particles:

$$Z_{GrandFermi}(T) = \sum_{n_1 n_2 n_3 \ldots\ldots} \exp(-\beta(n_1(\epsilon_1 - \mu) + n_2(\epsilon_2 - \mu) + n_3(\epsilon_3 - \mu)\ldots))$$

Here we sum over all occupation numbers n_s and energies ϵ_s.

For N particles, the occupation numbers have the condition

$$N = \sum_s n_s.$$

For Fermi particles n_s=0 or n_s=1 only

$$\ln\left(Z_{GrandFermi}(T)\right) = \sum_s \ln\left(1 + e^{-\beta(\epsilon_s - \mu)}\right)$$

$$\sum_s \frac{1}{e^{\beta(\epsilon_s - \mu)} + 1} = N$$

Summary of results for Bose particles

$$\ln\left(Z_{GrandBose}(T,\mu)\right) = -\sum_s \ln\left(1 - e^{-\beta(\epsilon_s - \mu)}\right)$$

$$\sum_s \frac{1}{e^{\beta(\epsilon_s-\mu)} - 1} = N$$

Summary of results for Fermi particles

$$\ln\left(Z_{GrandFermi}(T)\right) = \sum_s \ln\left(1 + e^{-\beta(\epsilon_s - \mu)}\right)$$

$$\sum_s \frac{1}{e^{\beta(\epsilon_s-\mu)} + 1} = N$$

Do you think that Fermi and Bose particles behave the same at low temperatures?

Fermi distribution function

$$\mathcal{F}(\epsilon_s) = \frac{1}{e^{\beta(\epsilon_s-\mu)}+1}$$