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

Record!!!

Discussion for Lecture 32:

Recap of Bose condensation; Treatment of particle interactions in statistical mechanics

Reading: Sections 7.6 and 8.1

1. **Recap of Bose condensate**
2. **Treatment and effects of interparticle interactions in statistical mechanics**

28	Fri: 04/09/2021	Chap. 7.3 & 7.4	Bose and Fermi statistics	#23	04/12/2021
29	Mon: 04/12/2021	Chap. 7.3	Fermi examples	#24	04/16/2021
30	Wed: 04/14/2021	Chap. 7.5	Bose examples and lattice vibrations		
31	Fri: 04/16/2021	Chap. 7.6	Bose condensation		
32	Mon: 04/19/2021	Chap. 7.6 & 8.1	Interacting particles	#25	04/21/2021
33	Wed: 04/21/2021	Chap. 8.1	Interacting particles		
34	Fri: 04/23/2021	Chap. 8.2	Spin magnetism		
35	Mon: 04/26/2021	Chap. 8.2	Spin magnetism		
36	Wed: 04/28/2021		Review		
37	Fri: 04/30/2021		Review		
37	Mon: 05/03/2021		Review		
38	Wed: 05/05/2021		Review		

PHY 341/641 -- Assignment #25

April 19, 2021

Complete Section 7.6 and start reading Section 8.1 in **Schroeder** .

Suppose that you have an ideal Bose gas of ^{87}Rb atoms with a number density of 2.5×10^{20} atoms/m^3. Each atom has a mass of 1.44×10^{-25} kg. Other constants that you may want to use for this problem are the Boltzmann constant of $k=1.380649 \times 10^{-23}$ J/K and Planck's constant of $h=6.62607015 \times 10^{-34}$ J s. Additionally, you will need to evaluate the function that we defined in class whose integral can be evaluated with software (Maple, Mathematica, etc.) or it can be evaluated from a convergent infinite series $g_{3/2}(z)=\sum_{m=1}^{\infty} z^m m^{-3/2}$.

1. Find the critical temperature T_c for forming a Bose condensate in this system.
2. Find the chemical potential for this system at T=0.00001 K.

Some review of Bose condensate -- Bose particles are characterized by integer intrinsic spin. In the following we will assume s=0. They have the property that there are no restrictions on the occupancy of each single particle state. Therefore, there is the possibility that there can be a macroscopic number of particles occupying the ground state (in our case at ε_0=0)

For temperatures below the critical temperature T_c there are N_0 particles in the ground state and the sum rule for the total number of particles of the system (ideal Bose particles in a three dimensional box of volume V) is

$$N = N_0 + \int_{0^+}^{\infty} d\epsilon g(\epsilon) \frac{1}{e^{\beta(\epsilon-\mu)} - 1} \quad \text{where } g(\epsilon) = 2\pi V \left(\frac{2m}{h^2}\right)^{3/2} \sqrt{\epsilon}$$

It is convenient to use the notation $z \equiv e^{\beta\mu}$.

$$N = N_0 + 2\pi V \left(\frac{2mkT}{h^2}\right)^{3/2} \int_{0^+}^{\infty} dx \frac{\sqrt{x}z}{e^x - z}$$

$$= N_0 + V\left(\frac{2\pi mkT}{h^2}\right)^{3/2} g_{3/2}(z) \qquad \text{where } g_{3/2}(z) \equiv \frac{2}{\sqrt{\pi}} \int_0^{\infty} dx \frac{z\sqrt{x}}{e^x - z} = \sum_{j=1}^{\infty} \frac{z^j}{j^{3/2}}$$

At the critical temperature T_c, N_0=0 and z=1 for $0 \leq T \leq T_c$

$$N = V\left(\frac{2\pi mkT_c}{h^2}\right)^{3/2} g_{3/2}(1)$$

For $0 \leq T \leq T_c$ --> $N = N_0 + V\left(\frac{2\pi mkT}{h^2}\right)^{3/2} g_{3/2}(1)$

$$\frac{N_0}{N} = 1 - \left(\frac{T}{T_c}\right)^{3/2}$$

For $T > T_c, \quad N_0 = 0$ and $z < 1$:

$$N = V\left(\frac{2\pi mkT}{h^2}\right)^{3/2} g_{3/2}(z) \quad \text{for } z < 1$$

$$\mu = kT\ln(z)$$

Note that $\mu = 0$ for $0 \le T \le T_c$

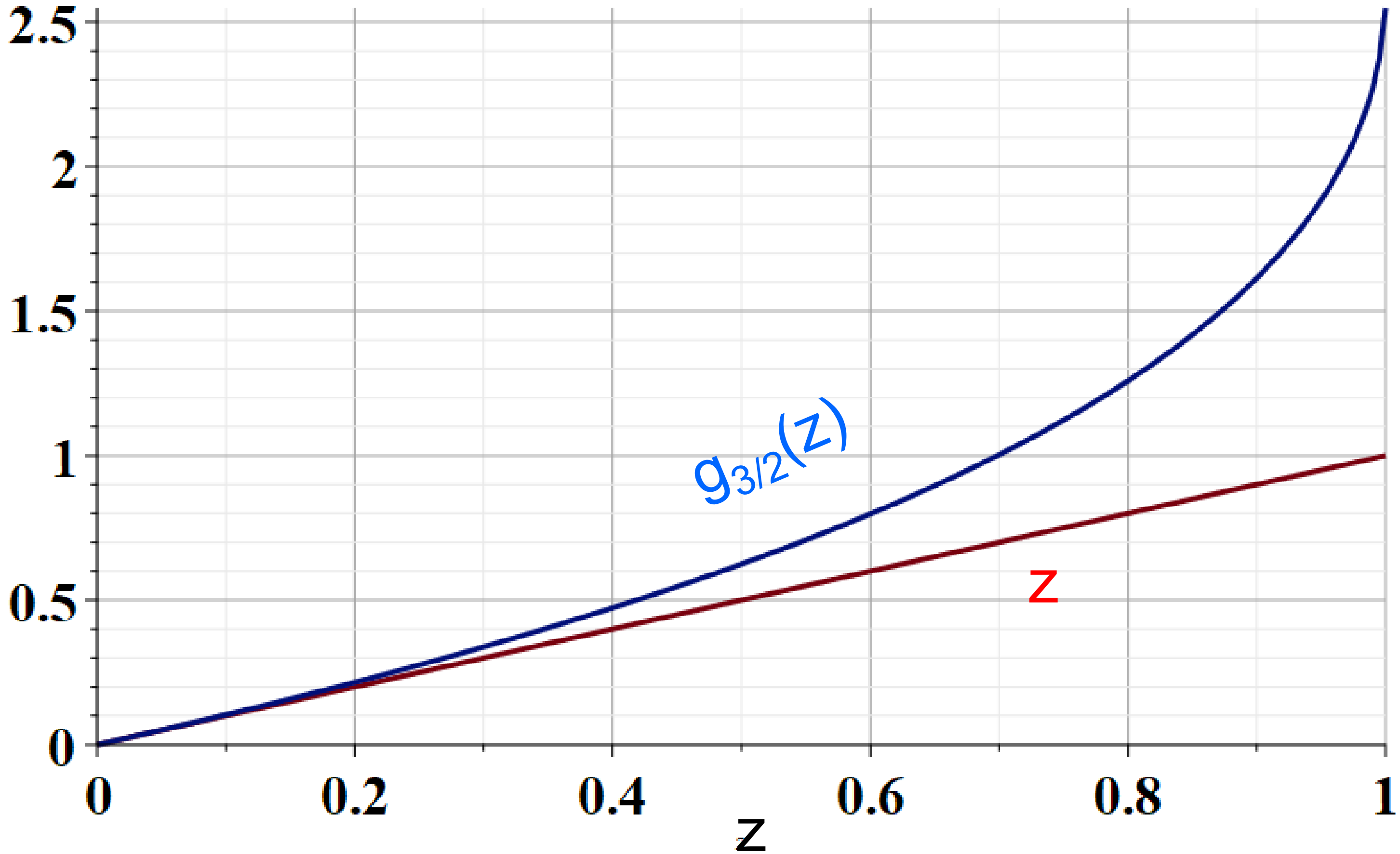
$\mu < 0$ for $T > T_c$

Behavior of Bose gas for $T >> T_c$

$$g_{3/2}(z) = \frac{N}{V}\left(\frac{h^2}{2\pi mkT}\right)^{3/2} \quad \text{where } g_{3/2}(z) = \sum_{j=1}^{\infty} \frac{z^j}{j^{3/2}}$$

Behavior of Bose gas for $T >> T_c$

$$g_{3/2}(z) = \frac{N}{V}\left(\frac{h^2}{2\pi mkT}\right)^{3/2} \qquad \text{where } g_{3/2}(z) = \sum_{j=1}^{\infty} \frac{z^j}{j^{3/2}}$$

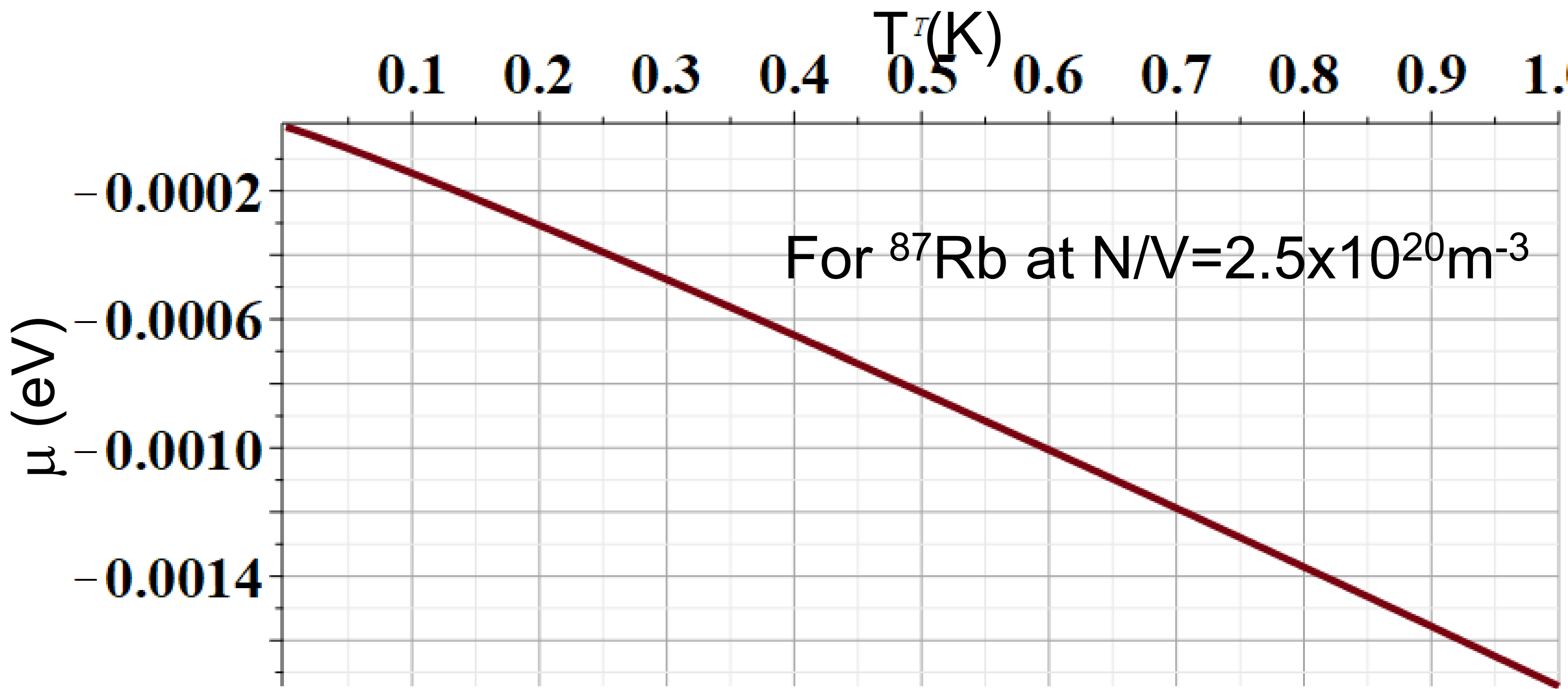


For $T >> T_c$

$$z \approx \frac{N}{V}\left(\frac{h^2}{2\pi mkT}\right)^{3/2}$$

$$\mu = kT \ln z \approx -kT \ln\left(\frac{V}{N}\left(\frac{2\pi mkT}{h^2}\right)^{3/2}\right)$$

Result for classical monoatomic ideal gas!



Your questions on Chap. 8

From Kristen -- 1. Why does the momentum (p) not appear in the first term of equations 8.2 and 8.4? 2. What is the Mayer f-function explicitly? 3. I understand where B(T) comes from mathematically, but does it have any physical representation outside of the formula?

From Rich -- What are the u0 and r0 constraints used in the equation 8.37?

From Michael --Our book mentions a symmetry factor, I was wondering if you could please expand on this a little bit, about what exactly it is and how we find it?

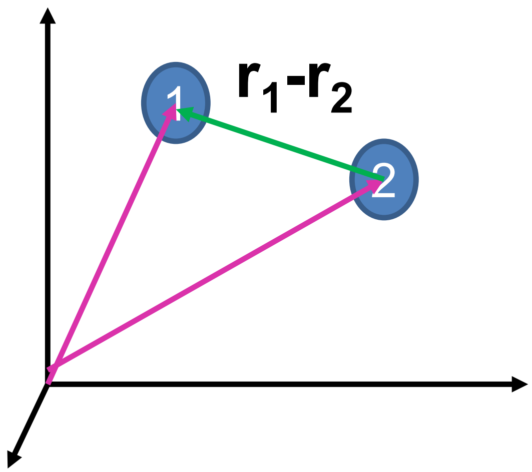
Up to now, we have focused on systems that can be well described as independent (non-interacting) particles. More realistically, particles do interact. Typically this interaction can be described in terms an interacting potential energy term. As an example, we will consider a gas of N monoatomic atoms of mass m treated using classical mechanics .

The classical Hamiltonian of the system has kinetic energy

and potential energy contributions: $\mathcal{H} = \sum_{i=1}^{N} \frac{|\mathbf{p}_i|^2}{2m} + \Phi(\mathbf{r}_1, \mathbf{r}_2 ..)$

We have been ignoring this term

Some typical potential interactions



Coulomb interaction

$$\Phi(|\mathbf{r}_1 - \mathbf{r}_2|) = \frac{q^2}{4\pi\epsilon_0} \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|}$$

Lennard-Jones interaction

$$\Phi(|\mathbf{r}_1 - \mathbf{r}_2|) = \Phi_0 \left(\left(\frac{r_0}{|\mathbf{r}_1 - \mathbf{r}_2|} \right)^{12} - 2 \left(\frac{r_0}{|\mathbf{r}_1 - \mathbf{r}_2|} \right)^6 \right)$$

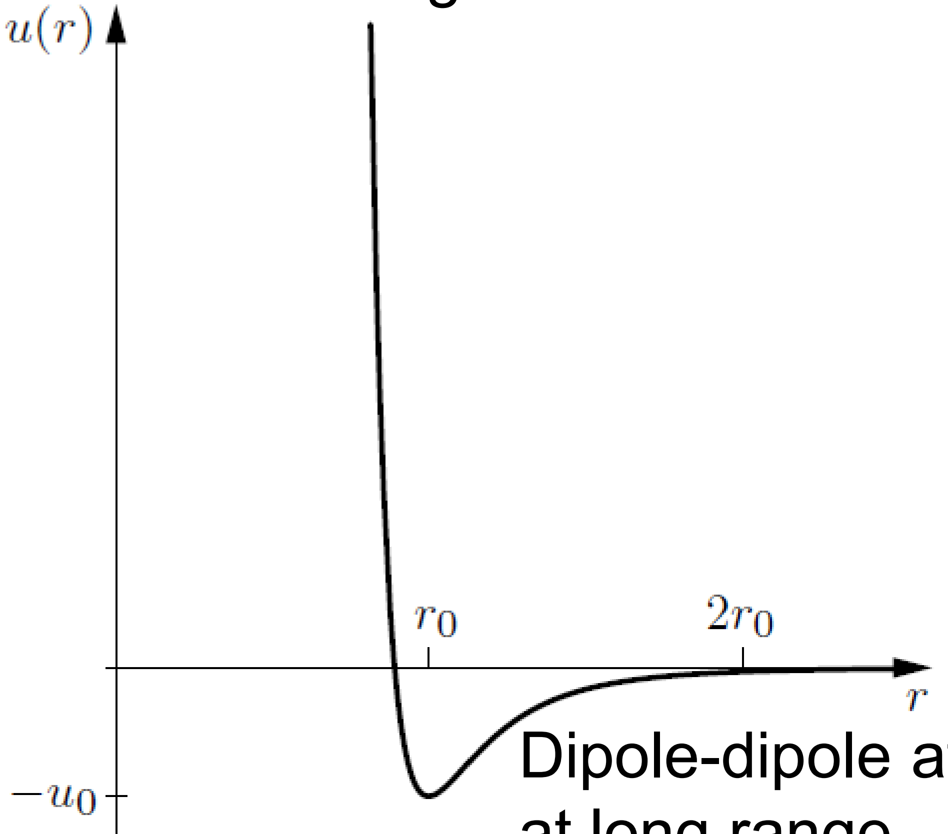
Born-Mayer potential

$$\Phi(|\mathbf{r}_1 - \mathbf{r}_2|) = \Phi_0 e^{-\lambda|\mathbf{r}_1 - \mathbf{r}_2|} + \frac{q^2}{4\pi\epsilon_0} \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|}$$

In practice, potential interactions can involve more than 2 particles and can be angularly dependent.

The Lennard-Jones pair potential does a good job of describing the interaction between rare gas atoms.

Repulsive interaction at short range



Dipole-dipole attraction at long range

Measured Lennard-Jones parameters for some rare gas atoms (Ref. Ashcroft and Mermin, Solid State Physics)

	Ne	Ar	Kr	Xe
U_0 (eV)	0.0031	0.0104	0.0140	0.0200
r_0 (Angstroms)	3.08	3.82	4.10	4.47

$$\Phi(\mathbf{r}_1, \mathbf{r}_2 \ldots) \approx \sum_{pairs\ (ij)} \phi_{pair}\left(\left|\mathbf{r}_i - \mathbf{r}_j\right|\right)$$

Classical canonical partition function for gas of particles of mass m in the presence of an interaction potential

$$Z(T,V,N)=\frac{1}{N!h^{3N}}\int d^3r_1 d^3r_2..d^3r_N d^3p_1 d^3p_2..d^3p_N e^{-\beta\mathcal{H}}$$

where $\mathcal{H}=\sum_{i=1}^{N}\frac{|\mathbf{p}_i|^2}{2m}+\Phi(\mathbf{r}_1,\mathbf{r}_2..)\equiv\mathcal{H}_{kin}+\Phi(\mathbf{r}_1,\mathbf{r}_2..)$

$$Z(T,V,N)=Z_{kin}(T,V,N)Z_{pot}(T,V,N)$$

$$Z_{kin}(T,V,N)\equiv\frac{V^N}{N!h^{3N}}\int d^3p_1 d^3p_2..d^3p_N e^{-\beta\mathcal{H}_{kin}}$$

$$=\frac{V^N}{N!}\left(\frac{2\pi mkT}{h^2}\right)^{3/2}$$

$$Z_{pot}(T,V,N)\equiv\frac{1}{V^N}\int d^3r_1 d^3r_2..d^3r_N e^{-\beta\Phi(\mathbf{r}_1,\mathbf{r}_2..)}$$

Evaluation of the potential contributions --

$$Z_{pot}(T,V,N) \equiv \frac{1}{V^N}\int d^3r_1 d^3r_2..d^3r_N e^{-\beta\Phi(\mathbf{r}_1,\mathbf{r}_2..)}$$

$$\mathbf{\Phi(r_1,r_2...)} \approx \sum_{pairs\ (ij)} \phi_{pair}(|\mathbf{r}_i - \mathbf{r}_j|)$$

$$Z_{pot}(T,V,N) \approx \frac{1}{V^N}\int d^3r_1 d^3r_2..d^3r_N \prod_{pairs(ij)} e^{-\beta\phi_{pair}(|\mathbf{r}_i-\mathbf{r}_j|)}$$

Suppose that $e^{-\beta\phi_{pair}(|\mathbf{r}_i-\mathbf{r}_j|)} \equiv 1+f_{ij}$ $\qquad f_{ij} = e^{-\beta\phi_{pair}(|\mathbf{r}_i-\mathbf{r}_j|)} - 1 \approx -\beta\phi_{pair}(|\mathbf{r}_i - \mathbf{r}_j|)$

Then $\prod_{pairs(ij)} e^{-\beta\phi_{pair}(|\mathbf{r}_i-\mathbf{r}_j|)} = (1+f_{12})(1+f_{13})...(1+f_{23})...(1+f_{N-1N})$

$$= 1 + \sum_{pairs(ij)} f_{ij} + \sum_{pairs(ij,kl)} f_{ij}f_{kl} + ...$$

Evaluation of potential terms continued --

$$Z_{pot}(T,V,N) \approx \frac{1}{V^N}\int d^3r_1 d^3r_2..d^3r_N \prod_{pairs(ij)} e^{-\beta\phi_{pair}(|\mathbf{r}_i-\mathbf{r}_j|)}$$

$$= Z^0_{pot}(T,V,N) + Z^{pairs}_{pot}(T,V,N) + Z^{double\ pairs}_{pot}(T,V,N) + \ldots$$

$$Z^0_{pot}(T,V,N) = \frac{1}{V^N}\int d^3r_1 d^3r_2..d^3r_N = 1$$

$$Z^{pairs}_{pot}(T,V,N) = \frac{1}{V^N}\int d^3r_1 d^3r_2..d^3r_N \sum_{pairs(ij)} f_{ij} = \frac{1}{2}\frac{N(N-1)}{V^2}\int d^3r_1 d^3r_2 f_{12}$$