Statistical Mechanics - Class Exercise 3

November 28, 2022

The basic integrals for ideal gas

$$N = \sum_r f(\epsilon_r - \mu) = \int_0^\infty g(\epsilon) f(\epsilon - \mu) \, d\epsilon$$

$$E = \sum_r \epsilon_r f(\epsilon_r - \mu) = \int_0^\infty g(\epsilon) \epsilon f(\epsilon - \mu) \, d\epsilon$$

$$\boldsymbol{Z} = \prod_r \mathcal{Z}^{(r)}, \quad \mathcal{Z}^{(r)} = \sum_n e^{-\beta(\epsilon_r - \mu)n_r} = \left(1 \pm e^{-\beta(\epsilon_r - \mu)}\right)^{\pm 1}$$

$$\ln(\boldsymbol{Z}) = \pm \sum_r \ln\left(1 \pm e^{-\beta(\epsilon_r - \mu)}\right) = \{\text{Integration by parts}\} = \beta \int_0^\infty \mathcal{N}(\epsilon) f(\epsilon - \mu) \, d\epsilon$$

$$P = \frac{1}{\beta} \frac{\partial \ln(\boldsymbol{Z})}{\partial V} = \frac{1}{\beta} \frac{\ln(\boldsymbol{Z})}{V} = \frac{1}{V} \int_0^\infty \mathcal{N}(\epsilon) f(\epsilon - \mu) \, d\epsilon$$

Exercise 3336 - Condensation for general dispersion

An ideal Bose gas consists of particles that have the dispersion relation $\epsilon = c|p|^s$ with $s > 0$. The gas is contained in a box that has volume V in d dimensions. The gas is maintained in a uniform temperature T.

1. Calculate the single particle density of states.
2. Find a condition involving s and d for the existence of Bose-Einstein condensation. In particular relate to relativistic ($s = 1$) and nonrelativistic ($s = 2$) particles in two dimensions.
3. Find the dependence of the number of particles N on the chemical potential μ.
4. Find the dependence of the total energy E on the chemical potential, and show how the pressure P is obtained from this result.
5. Find an expression for the heat capacity C_v. Show how this result can be expressed using N in the limit of infinite temperature.
6. Repeat item 1 for relativistic gas whose particles have finite mass such that their dispersion relation is $\epsilon = \sqrt{m^2c^4 + c^2p^2}$.
7. Consider a relativistic gas in $2D$. Find expressions for N and E and P. Should one expect Bose-Einstein condensation?

Answer

1. We have the dispersion relation $\epsilon = c|p|^s$

$$\rightarrow |p| = \left(\frac{\epsilon}{c}\right)^{\frac{1}{s}}$$

$$\mathcal{N}(\epsilon) = \int_{H<\epsilon} \frac{d^d x d^d p}{(2\pi)^d} = \frac{V}{(2\pi)^d} \int \cdots \int_{\sqrt{p_1^2+\cdots+p_d^2} \leq \left(\frac{\epsilon}{c}\right)^{\frac{1}{s}}} d^d p = \frac{V}{(2\pi)^d} \Omega_d \int_0^{\left(\frac{\epsilon}{c}\right)^{\frac{1}{s}}} p^{d-1} dp = \frac{V}{(2\pi)^d} \frac{\Omega_d}{d} \left(\frac{\epsilon}{c}\right)^{\frac{d}{s}}$$

$$\mathcal{N}(\epsilon) = \frac{1}{d} \frac{V}{(2\pi)^d} \frac{\Omega_d}{c^{\frac{d}{s}}} \epsilon^{\frac{d}{s}}$$

$$g(\epsilon) = \frac{\partial \mathcal{N}(\epsilon)}{\partial \epsilon} = \frac{1}{s} \frac{V}{(2\pi)^d} \frac{\Omega_d}{c^{\frac{d}{s}}} \epsilon^{\frac{d}{s}-1}$$

$$\rightarrow \mathcal{N}(\epsilon) = \frac{s}{d} g(\epsilon) \epsilon$$

2. We define $\alpha = \frac{d}{s}, c = \frac{1}{(2\pi)^d} \frac{\Omega_d}{s c^{\frac{d}{s}}}$

In general

$$N = \int_0^\infty g(\epsilon) f(\epsilon - \mu) d\epsilon = cV \int_0^\infty \frac{\epsilon^{\alpha-1}}{e^{\beta(\epsilon-\mu)} - 1} d\epsilon$$

For Bose-Einstein condensation we need that the integral will converge even for $\mu = 0$, and this happen for $\alpha > 1 \rightarrow d > s$.

For nonrelativistic $(s = 2)$ particles in 2D $d = s$, so the system will not exhibit BEC.

For relativistic $(s = 1)$ particles in 2D $d > s$, so the system can exhibit BEC.

3. Define $z = e^{\beta\mu}$

$$N = cV \int_0^\infty \frac{\epsilon^{\alpha-1}}{e^{\beta(\epsilon-\mu)} - 1} d\epsilon = \left\{ \begin{array}{c} x = \beta\epsilon \\ T dx = d\epsilon \end{array} \right\} = cVT^\alpha \int_0^\infty \frac{x^{\alpha-1}}{\frac{1}{z} e^x - 1} dx = cVT^\alpha F_\alpha(\beta\mu)$$

Where

$$F_\alpha(\beta\mu) = \Gamma(\alpha) Li_\alpha(z), \quad Li_\alpha(z) = \sum_{\ell=1}^\infty \frac{z^\ell}{\ell^\alpha}$$

4. To calculate the total energy E:

$$E = \int_0^\infty g(\epsilon) \epsilon f(\epsilon - \mu) d\epsilon = cV \int_0^\infty \frac{\epsilon^\alpha}{e^{\beta(\epsilon-\mu)} - 1} d\epsilon = cVT^{\alpha+1} F_{\alpha+1}(\beta\mu)$$

In the other side

$$\ln(Z) = \beta \int_0^\infty \mathcal{N}(\epsilon) f(\epsilon - \mu) d\epsilon = \frac{\beta}{\alpha} \int_0^\infty g(\epsilon) \epsilon f(\epsilon - \mu) d\epsilon = \frac{\beta}{\alpha} cVT^{\alpha+1} F_{\alpha+1}(\beta\mu) = \frac{\beta}{\alpha} E$$

We know that

$$P = \frac{1}{\beta} \frac{\partial \ln(Z)}{\partial V} = \frac{1}{\beta} \frac{\ln(Z)}{V} = \frac{1}{\alpha} \frac{E}{V}$$

5. The heat capacity C_v.

$$C_v = \left. \frac{\partial E}{\partial T} \right|_{V,N}$$

In the limit of infinite temperature can use Boltzmann approximation; in this limit $f(\epsilon-\mu)=e^{-\beta(\epsilon-\mu)}$

$$N=cV\int_0^\infty \epsilon^{\alpha-1}e^{-\beta(\epsilon-\mu)}d\epsilon=cVe^{\beta\mu}T^\alpha\int_0^\infty x^{\alpha-1}e^{-x}dx=cVe^{\beta\mu}T^\alpha\Gamma(\alpha)$$

$$E=cV\int_0^\infty \epsilon^{\alpha}e^{-\beta(\epsilon-\mu)}d\epsilon=cVe^{\beta\mu}T^{\alpha+1}\Gamma(\alpha+1)=cVe^{\beta\mu}T^{\alpha+1}\alpha\Gamma(\alpha)=\alpha NT$$

$$\to C_v=\left.\frac{\partial E}{\partial T}\right|_{V,N}=\alpha N$$

6. For relativistic gas with dispersion relation is $\epsilon=\sqrt{m^2c^4+c^2p^2}$.

$$\to|p|=\sqrt{\left(\frac{\epsilon}{c}\right)^2-m^2c^2}$$

$$\mathcal{N}(\epsilon)=\int_{H<\epsilon}\frac{d^dxd^dp}{(2\pi)^d}=\frac{V}{(2\pi)^d}\int\cdots\int_{\sqrt{p_1^2+\cdots+p_d^2}\le\sqrt{\left(\frac{\epsilon}{c}\right)^2-m^2c^2}}d^dp=\frac{V}{(2\pi)^d}\Omega_d\int_0^{\sqrt{\left(\frac{\epsilon}{c}\right)^2-m^2c^2}}p^{d-1}dp$$
$$=\frac{V}{(2\pi)^d}\frac{\Omega_d}{d}\left(\left(\frac{\epsilon}{c}\right)^2-m^2c^2\right)^{\frac{d}{2}}$$

$$g(\epsilon)=\frac{\partial\mathcal{N}(\epsilon)}{\partial\epsilon}=\frac{V}{(2\pi)^d}\Omega_d\left(\left(\frac{\epsilon}{c}\right)^2-m^2c^2\right)^{\frac{d}{2}-1}\frac{\epsilon}{c^2}$$

7. For relativistic gas in $2D$ the momentum $|p|\sim\epsilon\to\alpha=\frac{d}{s}=2$

$$\mathcal{N}(\epsilon)=\frac{1}{2}\frac{V}{2\pi c^2}\left(\epsilon^2-m^2c^4\right)$$

$$g(\epsilon)=\frac{\partial\mathcal{N}(\epsilon)}{\partial\epsilon}=\frac{V}{2\pi c^2}\epsilon$$

$$N=\frac{V}{2\pi c^2}\int_{mc^2}^\infty\frac{\epsilon}{e^{\beta(\epsilon-\mu)}-1}d\epsilon=\left\{\epsilon'=\epsilon-mc^2\right\}=\frac{V}{2\pi c^2}\int_0^\infty\frac{\epsilon'+mc^2}{e^{\beta(\epsilon'+mc^2-\mu)}-1}d\epsilon'=$$
$$=\frac{V}{2\pi c^2}T^2F_2\left(\frac{\mu-mc^2}{T}\right)+\frac{Vmc^2}{2\pi c^2}TF_1\left(\frac{\mu-mc^2}{T}\right)$$

even for

$$N=\frac{V}{2\pi c^2}\left[T^2F_2\left(\frac{\mu-mc^2}{T}\right)+mc^2TF_1\left(\frac{\mu-mc^2}{T}\right)\right]$$

In the same way

$$E=\frac{V}{2\pi c^2}\int_{mc^2}^\infty\frac{\epsilon^2}{e^{\beta(\epsilon-\mu)}-1}d\epsilon=\frac{V}{2\pi c^2}\int_0^\infty\frac{\epsilon'^2+2\epsilon'mc^2+m^2c^4}{e^{\beta(\epsilon'+mc^2-\mu)}-1}d\epsilon'$$
$$E=\frac{V}{2\pi c^2}\left[T^3F_3\left(\frac{\mu-mc^2}{T}\right)+2mc^2T^2F_2\left(\frac{\mu-mc^2}{T}\right)+m^2c^4TF_1\left(\frac{\mu-mc^2}{T}\right)\right]$$

For P we need to calculate $\ln(Z)$

$$\ln(Z) = \beta \int_0^\infty \mathcal{N}(\epsilon) f(\epsilon-\mu) d\epsilon = \beta \frac{V}{4\pi c^2} \int_{mc^2}^\infty \frac{\left(\epsilon^2 - m^2c^4\right)}{e^{\beta(\epsilon-\mu)}-1} d\epsilon$$

$$= \beta \frac{V}{4\pi c^2} \int_0^\infty \frac{\epsilon'^2 + 2\epsilon' mc^2}{e^{\beta(\epsilon'+mc^2-\mu)}-1} d\epsilon' = \beta \frac{V}{4\pi c^2} \left[T^3 F_3\left(\frac{\mu - mc^2}{T}\right) + 2mc^2T^2F_2\left(\frac{\mu-mc^2}{T}\right)\right]$$

$$P = \frac{1}{\beta}\frac{\ln(Z)}{V} = \frac{1}{4\pi c^2}\left[T^3 F_3\left(\frac{\mu - mc^2}{T}\right) + 2mc^2T^2F_2\left(\frac{\mu-mc^2}{T}\right)\right]$$

for get BEC we need that $N = \int_0^\infty g(\epsilon) f(\epsilon-\mu) d\epsilon$ will be finite for $\mu \to 0$

$$N = \frac{V}{2\pi c^2} \int_0^\infty \frac{\epsilon' + mc^2}{e^{\beta(\epsilon'+mc^2-\mu)}-1} d\epsilon' = \frac{V}{2\pi c^2} \int_0^\infty \frac{\epsilon' + mc^2}{e^{\beta(\epsilon'-\mu')}-1} d\epsilon'$$

For $\mu \to mc^2 \Leftrightarrow \mu' \to 0$ we get that $\int_0^\infty \frac{mc^2}{e^{\beta(\epsilon'-\mu')}-1} d\epsilon'$ does not converge and so we can't expect to get BEC. In another way we can see that for $\frac{p}{m} \ll c$

$$\epsilon = \sqrt{m^2c^4 + c^2p^2} \approx mc^2 + \frac{p^2}{2m} \to \alpha = 1$$

Exercise 3021 - Spin 1 bosons in 3D box with Zeeman interaction

N Bosons that have mass m and spin 1 are placed in a box that has volume V. A magnetic field B is applied, such that the interaction is $-\gamma B S_z$, where $S_z = 1, 0, -1$, and γ is the gyromagnetic ratio. In items (3-6) assume the Boltzmann approximation for the occupation of the $S_z \neq 1$ states.

1. Find an equation for the condensation temperature T_c.
2. Find the condensation temperature $T_c(B)$ for $B = 0$ and for $B \to \infty$.
3. Find the critical B for condensation if T is set in the range of temperatures that has been defined in item (2).
4. Describe how $T_c(B)$ depends of B in a qualitatively manner. Find approximate expressions for moderate and large fields.
5. Find the condensate fraction as a function of T and B.
6. Find the heat capacity of the gas assuming large but finite field.

Answer

1. The Hamiltonian for one particle:

$$H = \frac{p^2}{2m} - \gamma B S_z$$

For $\alpha = \frac{d}{s} = \frac{3}{2}, c = \frac{1}{(2\pi)^d}\frac{\Omega_d}{sc^{\frac{d}{s}}} = \frac{(2m)^{\frac{3}{2}}}{(2\pi)^2}$ For spinless particles we get

$$N = cVT^{\frac{3}{2}} F_{3/2}(\beta\mu) = V \frac{2^{\frac{3}{2}} \left(\frac{mT}{2\pi}\right)^{\frac{3}{2}}}{(2\pi)^{\frac{1}{2}}} \Gamma\left(\frac{3}{2}\right) Li_{3/2}\left(e^{\beta\mu}\right) = \frac{V}{\lambda_T^3} Li_{3/2}\left(e^{\beta\mu}\right)$$

we can treat the particles of the system like three different spinless gasses with different S_z.

$$N = \sum f(\epsilon - \mu) = \sum f\left(\frac{p^2}{2m} - \gamma B - \mu\right) + \sum f\left(\frac{p^2}{2m} - \mu\right) + \sum f\left(\frac{p^2}{2m} + \gamma B - \mu\right)$$

We can define $\mu' = \mu + \gamma B S_z$ and get

$$\frac{N}{V} = \frac{1}{\lambda_T^3}\left(\mathrm{Li}_{3/2}\left(e^{\beta(\mu+\gamma B)}\right) + \mathrm{Li}_{3/2}\left(e^{\beta\mu}\right) + \mathrm{Li}_{3/2}\left(e^{\beta(\mu-\gamma B)}\right)\right)$$

The condition to condensation is that μ goes to the lowest energy, here this mean $\mu \to -\gamma B$ ($S_z = 1$)

$$\frac{N}{V} = n = n_0 + \frac{1}{\lambda_T^3}\left(\mathrm{Li}_{3/2}(1) + \mathrm{Li}_{3/2}\left(e^{-\beta\gamma B}\right) + \mathrm{Li}_{3/2}\left(e^{-2\beta\gamma B}\right)\right)$$

For $T = T_c$

$$n \approx \frac{1}{\lambda_T^3}\left(\zeta\left(\frac{3}{2}\right) + \mathrm{Li}_{3/2}\left(e^{-\beta\gamma B}\right) + \mathrm{Li}_{3/2}\left(e^{-2\beta\gamma B}\right)\right), \quad \zeta\left(\frac{3}{2}\right) \approx 2.612$$

2. For $B = 0$

$$n = \frac{1}{\lambda_T^3}\left(\mathrm{Li}_{3/2}(1) + \mathrm{Li}_{3/2}(1) + \mathrm{Li}_{3/2}(1)\right) = \frac{3}{\lambda_T^3}\zeta\left(\frac{3}{2}\right) = \underbrace{3}_{\text{spin}} \times \left(\frac{m}{2\pi}\right)^{\frac{3}{2}} \zeta\left(\frac{3}{2}\right) T_c^{\frac{3}{2}}$$

$$\to T_c(B=0) = \frac{2\pi}{m}\left(\frac{n}{3 \cdot 2.612}\right)^{\frac{2}{3}}$$

For $B \to \infty$ the occupation states are just $S_z = 1$, we get $\mathrm{Li}_{3/2}\left(e^{-\beta\gamma B}\right) \to 0$

$$n = \left(\frac{m}{2\pi}\right)^{\frac{3}{2}} \zeta\left(\frac{3}{2}\right) T_c^{\frac{3}{2}}$$

$$\to T_c(B=\infty) = \frac{2\pi}{m}\left(\frac{n}{2.612}\right)^{\frac{2}{3}}$$

$$\frac{T_c(B=\infty)}{T_c(B=0)} = 3^{\frac{2}{3}} \approx 2$$

3. Now we assume $B \neq 0$, $\gamma B \gg T$, so for $S_z \neq 1$ we can use the Boltzmann approximation.

$$n \approx \frac{1}{\lambda_T^3}\left(\mathrm{Li}_{3/2}(1) + e^{-\beta\gamma B} + e^{-2\beta\gamma B}\right) \approx \frac{1}{\lambda_T^3}\left(\zeta\left(\frac{3}{2}\right) + e^{-\beta\gamma B}\right)$$

$$\to B_c = -\frac{T}{\gamma}\ln\left(\lambda_T^3 n - \zeta\left(\frac{3}{2}\right)\right)$$

4. As B is increased, T_c rises until B_c is reached. At $B = B_c, T = T_c$ and the condensation occurs

$$n = \left(\frac{m}{2\pi}\right)^{\frac{3}{2}} T_c^{\frac{3}{2}} \left(\zeta\left(\frac{3}{2}\right) + e^{-\beta\gamma B}\right)$$

5. We get

$$n_0 = n - \frac{1}{\lambda_T^3}\left(\zeta\left(\frac{3}{2}\right) + e^{-\beta\gamma B}\right)$$

So

$$\frac{n_0}{n} = 1 - \frac{\left(\zeta\left(\frac{3}{2}\right) + e^{-\beta\gamma B}\right)}{n\lambda_T^3} = 1 - \frac{n\left(T, B\right)}{n}$$

6. For large but finite field $\gamma B \gg T$

$$\frac{E}{V} = \frac{3}{2}\frac{T}{\lambda_T^3}\left(\mathrm{Li}_{5/2}\left(1\right) + e^{-\beta\gamma B} + e^{-2\beta\gamma B}\right) \approx \frac{3}{2}\left(\frac{m}{2\pi}\right)^{\frac{3}{2}} T^{\frac{5}{2}}\left(\zeta\left(\frac{5}{2}\right) + e^{-\frac{\gamma B}{T}}\right)$$

$$\frac{C_V}{V} = \frac{\partial}{\partial T}\left(\frac{E}{V}\right) = \frac{3}{2}\frac{1}{\lambda_T^3}\left[\frac{5}{2}\zeta\left(\frac{5}{2}\right) + \left(\frac{5}{2} + \beta\gamma B\right)e^{-\beta\gamma B}\right] \approx \frac{3}{2}\frac{1}{\lambda_T^3}\left[\frac{5}{2}\zeta\left(\frac{5}{2}\right) + \beta\gamma B e^{-\beta\gamma B}\right]$$