Stat Mech Winter 2014

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1. Consider a classical ideal gas of N particles in three dimensions confined to an external potential $V(r) = K(r/r_0)^\alpha$, where $K > 0$, $\alpha > 0$, and $r_0 > 0$ are constants.
   (a) Show that the heat capacity is $C = \left(\frac{3}{2} + \frac{3}{2}\right) Nk$.
   (b) Suppose the shape of the parameter of the potential α may be varied. Why is it that the standard heat capacity of the free ideal gas $C_V = \frac{3}{2}Nk$ occurs in the limit $\alpha \to \infty$?

(a) The easiest way to find the heat capacity in this case is to use the overall method of

$$C_V = k\beta^2 \left(\frac{\partial^2}{\partial\beta^2}\right)_V \ln Z$$

Hence to find Z

$$\begin{aligned}
Z_1 &= \frac{4\pi}{h^3} \int_{\infty}^{\infty} d^3p \int_0^\infty dr\ r^2 e^{-\beta\left(\frac{p^2}{2m}\right)} e^{-\beta K\left(\frac{r}{r_0}\right)^\alpha} \\
&= \frac{4\pi}{h^3} \left(\frac{2\pi m}{\beta}\right)^{3/2} \int_0^\infty dr\ r^2 e^{-\beta K\left(\frac{r}{r_0}\right)^\alpha}
\end{aligned}$$

To extract the temperature dependence, we must convert this to a dimensionless integral using $x = (\beta K)^{1/\alpha} \frac{r}{r_0}$

$$\int_0^\infty dr\ r^2 e^{-\beta K\left(\frac{r}{r_0}\right)^\alpha} = (\beta K)^{-3/\alpha} r_0^3 \int_0^\infty d\left(\frac{(\beta K)^{1/\alpha} r}{r_0}\right) \left(\frac{(\beta K)^{1/\alpha} r}{r_0}\right)^2 e^{\left(\frac{(\beta K)^{1/\alpha} r}{r_0}\right)^\alpha}.$$

If we denote the dimensionless integral by I, then we have

$$Z_1 = \frac{4\pi}{h^3}(2\pi m)^{3/2} \beta^{-(3/2+3/\alpha)} K^{-3/\alpha} r_0^3$$

and so

$$\begin{aligned}
\ln Z = N \ln Z_1 = N \ln\gamma - N\left(\frac{3}{2} + \frac{3}{\alpha}\right)\ln(\beta) + \ln r_0^3 \\
k\beta^2 \frac{\partial}{\partial 2 * \beta} \ln Z = k\beta^2 \left(\frac{3}{2} + \frac{3}{\alpha}\right)\frac{1}{\beta^2} = \left(\frac{3}{2} + \frac{3}{\alpha}\right) Nk.
\end{aligned}$$

(b) If we look at the potential

$$\lim_{\alpha\to\infty} V(r) = \begin{cases} 0 & r < r_0 \\ \infty & r > r_0 \end{cases}$$

and so we end up confined in a bound box of dimension r_0^3. Hence we recover the usual heat capacity.

2. (a) For the two dimensional non-relativistic Bose gas with zero spin, calculate the chemical potential as a function of temperature and (area) density.
   (b) Do we have critical density and do we need to add Bose-Einstein condensate at low temperatures, as in the case of the three dimensional Bose gas?

(a) Dealing with Bosons, we are used to knowing the grand partition function and occupancy. A way to extract the chemical potential is to calculate N for this 2D gas. This can be done by integration. Remember that

$$\langle n_{\mathbf{k}} \rangle_B = \frac{1}{e^{\beta(\epsilon_k - \mu)} - 1}$$

so in the limit of continuation

$$N = \frac{L^2}{2\pi} \int_0^\infty dk \, \frac{k}{e^{\beta(\epsilon_k - \mu)} - 1}$$

Since it is nonrelativistic, the dispersion relation is

$$\epsilon(\mathbf{k}) = \frac{\hbar^2 |\mathbf{k}|^2}{2m}$$

and

$$d\epsilon = dk \frac{\hbar^2}{m} k$$

$$k = \sqrt{\frac{2m\epsilon}{\hbar^2}}$$

so

$$k \; dk = \frac{m}{\hbar^2} d\epsilon.$$

While we are here, we might as well generalize this for D dimension for part (b). The density relations are

$$k^{D-1} dk = k^{D-2} \, \frac{m}{\hbar^2} d\epsilon = \left(\frac{2m\epsilon}{\hbar^2}\right)^{(D-2)/2} \frac{m}{\hbar^2} \, d\epsilon = \frac{1}{2} \left(\frac{2m}{\hbar^2}\right)^{D/2} \epsilon^{(D-2)/2} \; d\epsilon.$$

Back to the 2D integral

$$\begin{aligned}
\int_0^\infty dk \, \frac{k}{e^{\beta(\epsilon_k - \mu)} - 1} &= \frac{m}{\hbar^2} \int_0^\infty d\epsilon \, \frac{1}{e^{\beta(\epsilon - \mu)} - 1} \\
&= \frac{m}{\hbar^2 \beta} \int_{-\beta\mu}^\infty d(\beta(\epsilon - \mu)) \frac{1}{e^{\beta(\epsilon - \mu)} - 1} \\
&= \frac{m}{\hbar^2 \beta} \int_{-\beta\mu}^\infty d(\beta(\epsilon - \mu)) \frac{e^{-\beta(\epsilon - \mu)}}{1 - e^{-\beta(\epsilon - \mu)}} \\
&= \frac{m}{\hbar^2 \beta} \int_{-\beta\mu}^\infty d(\beta(\epsilon - \mu)) \; \frac{\partial}{\partial(\beta(\epsilon - \mu))} \ln(1 - e^{-\beta(\epsilon - \mu)}) \\
&= \frac{m}{\hbar^2 \beta} \ln(1 - e^{-\beta(\epsilon - \mu)}) \Big|_{-\beta\mu}^\infty \\
&= -\frac{m}{\hbar^2 \beta} \ln\left(1 - e^{\beta\mu}\right)
\end{aligned}$$

Gathering the rest of the constants we have

$$N = -\frac{L^2}{2\pi} \left(\frac{m}{\hbar^2 \beta}\right) \ln(1 - e^{\beta\mu})$$

solving for μ

$$\mu = kT \ln\left(1 - e^{-\frac{2\pi\hbar^2 \beta n}{m}}\right)$$

This suggests that $-\infty < \mu < 0$, which, upon further reading, is not crazy. This means the system actually loses free energy as another particle input i.e., you have to do work to extract a particle out of the system. This is characteristic to bosons. With fermions, it takes work to input a particle.

(b) For a fixed temperature, the critical density is defined as the density at which

$$N_E(T, \mu = \epsilon_0) = N_C$$

In this notation, it is the density of excited states (given by the integral) at $\mu = \epsilon_0$ where $\epsilon_0 = 0$ in our case. It is the maximum density of the excited states. However, as we let $\mu \to \epsilon_0$ the ground state

$$\langle n_0 \rangle = \frac{1}{e^{\beta(\epsilon_0 - \mu)} - 1}$$

becomes macroscopically large. If we assume that the chemical potential calculated in part (a) is the density of the excited states, then the critical density is given when $\mu = 0$ which leads to

$$\ln\left(1 - \exp\left(-\frac{2\pi\hbar^2 n}{kT}\right)\right) = 0.$$

For a fixed temperature, this happens when

$$n \to \infty.$$

However, it seems that we have no way of separating the ground state from the

3. For a non-realtivistic ideal degenerate ($T = 0$) Fermi gas, find the average relative velocity $|\mathbf{v}_1 - \mathbf{v}_2|$ of the two particles.

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4. The dynamics of the vibrational normal modes of a solid made of N atoms can be approximated in terms of uncoupled harmonic oscillators by the Hamiltonian

$$H = \sum_{j=1}^{3N} \frac{p_j^2}{2m} + \frac{1}{2} m\omega_j^2 x_j^2.$$

(a) Calculate the canonical partition function $Z(T, N)$ of the system, determine its internal energy U, and show that it can be written as

$$U(T, N) = \int_0^\infty \frac{1}{2}\hbar\omega \coth\left(\frac{1}{2}\beta\hbar\omega\right) \sigma(\omega) d\omega$$

with the normal-mode vibrational frequency distribution $\sigma(\omega) = \sum_{j=1}^{3N} \delta(\omega - \omega_j)$.

(b) Consider the Einstein model of a solid where $\sigma(\omega) = \sum_{j=1}^{3N} \delta(\omega - \omega_j)$ with $\omega_j = \omega_E \ \forall \ j$. Derive the expression for the heat capacity C. Show that C satisfies the Dulong-Petit law for $T \gg T_E$, and vanishes exponentially for $T \ll T_E$ where $T_E = \hbar\omega_E / k_B$.

(c) Consider the Debye model which assumes $\sigma(\omega) = 9N\omega^2/\omega_D^2$ if $\omega \leq \omega_D$ and zero otherwise, where the value of ω_D is fixed by the normalization condition $\int_0^\infty \sigma(\omega)\, d\omega = 3N$. Derive the expression for the heat capacity C. Show that C satisfies the Dulong-Petit law for $T \gg T_D$, and vanishes like $C = const \times T^n$ for $T \ll T_D$ where $T_D = \hbar\omega_D / k_B$.
Remark: your calculation should determine the power n.
Hint: you may encounter an integral of the type $\int_0^\infty dx\ x^4 e^x/(e^x - 1)^2 = \frac{4\pi^4}{15}$.

(d) What does the third law of thermodynamics imply for the heat capacity? Do the models of Einstein and Debye discussed in part (b) and (c) satisfy the third law of thermodynamics?