PHYSICS 210A : EQUILIBRIUM STATISTICAL PHYSICS
HW ASSIGNMENT #4 SOLUTIONS

(1) Consider a three dimensional gas of particles with dispersion $\varepsilon(\boldsymbol{k}) = \varepsilon_0 (ka)^{3/2}$, where ε_0 and a are microscopic energy and length scales, respectively.

(a) Find the density of states per unit volume $g(\varepsilon)$. You may assume there are no internal degeneracies.

(b) Find an expression for the expansion coefficients $C_j(T)$ defined in eqn. 5.33 of the lecture notes.

(c) Find the virial coefficients $B_j(T)$ up through $j = 5$. It is convenient to use the `Mathematica` function `InverseSeries`. For guidance, see example problem 5.13.

Solution :

(a) For the general power law dispersion $\varepsilon(\boldsymbol{k}) = \varepsilon_0 (ka)^\sigma$ we have

$$k(\varepsilon) = \frac{1}{a}\left(\frac{\varepsilon}{\varepsilon_0}\right)^{1/\sigma} \qquad , \qquad k'(\varepsilon) = \frac{1}{\sigma a}\,\varepsilon_0^{-1/\sigma}\,\varepsilon^{-1-(1/\sigma)} \quad .$$

From $g(\varepsilon) = k^2(\varepsilon)\,k'(\varepsilon)/4\pi^2$ we then obtain

$$g(\varepsilon) = \frac{\varepsilon^{(3/\sigma)-1}}{4\pi^2 \sigma a^3 \varepsilon_0^{3/\sigma}} \quad .$$

(b) We have

$$C_j(T) = (\pm 1)^{j-1} \int_0^\infty \! d\varepsilon \; g(\varepsilon)\, e^{-j\varepsilon/k_B T} = (\pm 1)^{j-1} \lambda_T^{-3}\, j^{-3/\sigma}$$

where we define λ_T through

$$\lambda_T^3 \equiv \frac{4\pi^2 \sigma a^3}{\Gamma(3/\sigma)} \left(\frac{\varepsilon_0}{k_B T}\right)^{3/\sigma} \quad .$$

(c) With $\sigma = \frac{3}{2}$ we have $\frac{3}{\sigma} = 2$ and thus for bosons we have

$$\begin{aligned} n\lambda_T^3 &= z + 2^{-3\sigma^{-1}} z^2 + 3^{-3\sigma^{-1}} z^3 + + 4^{-3\sigma^{-1}} z^4 + \ldots \\ \beta p \lambda_T^3 &= z + 2^{-(3\sigma^{-1}+1)} z^2 + 3^{-(3\sigma^{-1}+1)} z^3 + 4^{-(3\sigma^{-1}+1)} z^4 + \ldots \quad . \end{aligned}$$

With $\sigma = \frac{3}{2}$ we have $\frac{3}{\sigma} = 2$. We now use the handy `Mathematica` function `InverseSeries` to obtain

```
In[1]=  y = InverseSeries[z + z^2/2^2 + z^3/3^2 + z^4/4^2 + z^5/5^2 + O[z]^6]
```

$$\text{Out[1]=}\quad x - \frac{x^2}{4} + \frac{x^3}{72} - \frac{x^4}{576} - \frac{31\,x^5}{86\,400} + O[x]^6$$

```
In[2]=  w = y + y^2/2^3 + y^3/3^3 + y^4/4^3 + y^5/5^3
```

$$\text{Out[2]=}\quad x - \frac{x^2}{8} - \frac{5\,x^3}{432} - \frac{x^4}{384} - \frac{2069\,x^5}{2\,592\,000} + O[x]^6$$

We may now read off the bosonic virial coefficients. For the fermionic case, we reverse the sign of the even coefficients. Thus

$$B_2(T) = \mp\tfrac{1}{8}\,\lambda_T^3 \quad , \quad B_3(T) = -\tfrac{5}{432}\,\lambda_T^6 \quad , \quad B_4(T) = \mp\tfrac{1}{384}\,\lambda_T^9 \quad , \quad B_5(T) = -\tfrac{2069}{2592000}\,\lambda_T^{12} \quad .$$

(2) In our derivation of the low temperature phase of an ideal Bose condensate, we split off the lowest energy state ε_0 but treated the remainder as a continuum, taking $\mu = 0$ in all expressions relating to the overcondensate. Under what conditions is this justified? *I.e.* why are we not obligated to separately consider the contributions from the first excited state, *etc.*?

Solution :

In the condensed phase, there is an extensive population N_0 of the lowest single particle energy state, and the chemical potential takes the value $\mu = \varepsilon_0 - \frac{k_B T}{g_0 N_0}$, where g_0 is the degeneracy of the single particle ground state. Let ε_1 be the energy of the first excited state and g_1 its degeneracy. Then the number of bosons in the first excited state is

$$N_1 = \frac{g_1}{e^{(\varepsilon_1 - \mu)/k_B T} - 1} \approx \frac{g_1 k_B T}{\varepsilon_1 - \mu} ,$$

assuming $\varepsilon_1 - \mu \ll k_B T$. Now

$$\varepsilon_1 - \mu = (\varepsilon_0 - \mu) + (\varepsilon_1 - \varepsilon_0) = \frac{k_B T}{g_0 N_0} + (\varepsilon_1 - \varepsilon_0) .$$

So we need to ask about the energy difference $\Delta\varepsilon_1 \equiv \varepsilon_1 - \varepsilon_0$. If $\Delta\varepsilon_1 \propto V^{-r}$, assuming $0 < r < 1$, then the number of particles in the first excited state will be subextensive, and the corresponding density $n_1 = N_1/V \propto V^{r-1}$ will vanish in the thermodynamic limit. In this case, we are justified in singling out only the single particle ground state as having an extensive occupancy. For a ballistic dispersion and periodic boundary conditions, the quantized single particle plane wave energies are given by

$$\varepsilon(l_x, l_y, l_z) = \frac{\hbar^2}{2m}\left\{\left(\frac{2\pi l_x}{L_x}\right)^2 + \left(\frac{2\pi l_y}{L_y}\right)^2 + \left(\frac{2\pi l_z}{L_z}\right)^2\right\},$$

and thus $\varepsilon_1 \propto V^{-2/3}$. Therefore $r = \frac{2}{3}$ and the occupancy of the first excited state is subextensive.

(3) Consider a three-dimensional Bose gas of particles which have two internal polarization states, labeled by $\sigma = \pm 1$. The single particle energies are given by

$$\varepsilon(\boldsymbol{p}, \sigma) = \frac{\boldsymbol{p}^2}{2m} + \sigma\Delta ,$$

where $\Delta > 0$.

(a) Find the density of states per unit volume $g(\varepsilon)$.

(b) Find an implicit expression for the condensation temperature $T_c(n, \Delta)$. When $\Delta \to \infty$, your expression should reduce to the familiar one derived in class.

(c) When $\Delta = \infty$, the condensation temperature should agree with the familiar result for three-dimensional Bose condensation. Assuming $\Delta \gg k_B T_c(n, \Delta = \infty)$, find analytically the leading order difference $T_c(n, \Delta) - T_c(n, \Delta = \infty)$.

Solution :

(a) Let $g_0(\varepsilon)$ be the DOS per unit volume for the case $\Delta = 0$. Then

$$g_0(\varepsilon)\, d\varepsilon = \frac{d^3k}{(2\pi)^3} = \frac{k^2\, dk}{2\pi^2} \quad \Rightarrow \quad g_0(\varepsilon) = \frac{1}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{1/2} \varepsilon^{1/2}\, \Theta(\varepsilon) .$$

For finite Δ, the single particle energies are shifted uniformly by $\pm\Delta$ for the $\sigma = \pm 1$ states, hence

$$g(\varepsilon) = g_0(\varepsilon + \Delta) + g_0(\varepsilon - \Delta) .$$

(b) For Bose statistics, we have in the uncondensed phase,

$$\begin{aligned} n &= \int\limits_{-\infty}^{\infty} d\varepsilon\, \frac{g(\varepsilon)}{e^{(\varepsilon-\mu)/k_B T} - 1} \\ &= \mathrm{Li}_{3/2}\big(e^{(\mu+\Delta)/k_B T}\big)\, \lambda_T^{-3} + \mathrm{Li}_{3/2}\big(e^{(\mu-\Delta)/k_B T}\big)\, \lambda_T^{-3} . \end{aligned}$$

In the condensed phase, $\mu = -\Delta - \mathcal{O}(N^{-1})$ is pinned just below the lowest single particle energy, which occurs for $\boldsymbol{k} = \boldsymbol{p}/\hbar = 0$ and $\sigma = -1$. We then have

$$n = n_0 + \zeta(3/2)\, \lambda_T^{-3} + \mathrm{Li}_{3/2}\big(e^{-2\Delta/k_B T}\big)\, \lambda_T^{-3} .$$

To find the critical temperature, set $n_0 = 0$ and $\mu = -\Delta$:

$$n = \zeta(3/2)\,\lambda_{T_c}^{-3} + \mathrm{Li}_{3/2}\big(e^{-2\Delta/k_B T_c}\big)\,\lambda_{T_c}^{-3}\ .$$

This is a nonlinear and implicit equation for $T_c(n,\Delta)$. When $\Delta = \infty$, we have

$$k_B T_c^{\infty}(n) = \frac{2\pi\hbar^2}{m}\left(\frac{n}{\zeta(3/2)}\right)^{2/3}\ .$$

(c) For finite Δ, we still have the implicit nonlinear equation to solve, but in the limit $\Delta \gg k_B T_c$, we can expand $T_c(\Delta) = T_c^{\infty} + \delta T_c(\Delta)$. We may then set $T_c(n,\Delta)$ to $T_c^{\infty}(n)$ in the second term of our nonlinear implicit equation, move this term to the LHS, whence

$$\zeta(3/2)\,\lambda_{T_c}^{-3} \approx n - \mathrm{Li}_{3/2}\big(e^{-2\Delta/k_B T_c^{\infty}}\big)\,\lambda_{T_c^{\infty}}^{-3}\ .$$

which is a simple algebraic equation for $T_c(n,\Delta)$. The second term on the RHS is tiny since $\Delta \gg k_B T_c^{\infty}$. We then find

$$T_c(n,\Delta) = T_c^{\infty}(n)\left\{1 - \tfrac{3}{2}\,e^{-2\Delta/k_B T_c^{\infty}(n)} + \mathcal{O}\big(e^{-4\Delta/k_B T_c^{\infty}(n)}\big)\right\}\ .$$

(4) A branch of excitations for a three-dimensional system has a dispersion $\varepsilon(\boldsymbol{k}) = A\,|\boldsymbol{k}|^{2/3}$. The excitations are bosonic and are not conserved; they therefore obey photon statistics.

(a) Find the single excitation density of states per unit volume, $g(\varepsilon)$. You may assume that there is no internal degeneracy for this excitation branch.

(b) Find the heat capacity $C_V(T,V)$.

(c) Find the ratio E/pV.

(d) If the particles are bosons with number conservation, find the critical temperature T_c for Bose-Einstein condensation.

Solution:

(a) We have, for three-dimensional systems,

$$g(\varepsilon) = \frac{1}{2\pi^2}\,\frac{k^2}{d\varepsilon/dk} = \frac{3}{4\pi^2 A}\,k^{7/3}\ .$$

Inverting the dispersion to give $k(\varepsilon) = (\varepsilon/A)^{3/2}$, we obtain

$$g(\varepsilon) = \frac{3}{4\pi^2}\,\frac{\varepsilon^{7/2}}{A^{9/2}}$$

(b) The energy is then

$$
\begin{aligned}
E &= V\int\limits_0^\infty d\varepsilon\; g(\varepsilon)\,\frac{\varepsilon}{e^{\varepsilon/k_{\rm B}T}-1} \\
&= \frac{3V}{4\pi^2}\,\Gamma\big(\tfrac{11}{2}\big)\,\zeta\big(\tfrac{11}{2}\big)\,\frac{(k_{\rm B}T)^{11/2}}{A^{9/2}}\ .
\end{aligned}
$$

Thus,

$$
C_V = \bigg(\frac{\partial E}{\partial T}\bigg)_V = \frac{3V}{4\pi^2}\,\Gamma\big(\tfrac{13}{2}\big)\,\zeta\big(\tfrac{11}{2}\big)\,k_{\rm B}\,\bigg(\frac{k_{\rm B}T}{A}\bigg)^{9/2}
$$

(c) The pressure is

$$
\begin{aligned}
p = -\frac{\Omega}{V} &= -k_{\rm B}T\int\limits_0^\infty d\varepsilon\; g(\varepsilon)\;\ln\big(1-e^{-\varepsilon/k_{\rm B}T}\big) \\
&= -k_{\rm B}T\int\limits_0^\infty d\varepsilon\;\frac{3}{4\pi^2}\,\frac{\varepsilon^{7/2}}{A^{9/2}}\;\ln\big(1-e^{-\varepsilon/k_{\rm B}T}\big) \\
&= -\frac{3}{4\pi^2}\,\frac{(k_{\rm B}T)^{11/2}}{A^{9/2}}\int\limits_0^\infty ds\; s^{7/2}\;\ln\big(1-e^{-s}\big) \\
&= \frac{3V}{4\pi^2}\,\Gamma\big(\tfrac{9}{2}\big)\,\zeta\big(\tfrac{11}{2}\big)\,\frac{(k_{\rm B}T)^{11/2}}{A^{9/2}}\ .
\end{aligned}
$$

Thus,

$$
\frac{E}{pV} = \frac{\Gamma\big(\frac{11}{2}\big)}{\Gamma\big(\frac{9}{2}\big)} = \tfrac{9}{2}
$$

(d) To find $T_{\rm c}$ for BEC, we set $z=1$ (*i.e.* $\mu=0$) and $n_0=0$, and obtain

$$
n = \int\limits_0^\infty d\varepsilon\; g(\varepsilon)\,\frac{\varepsilon}{e^{\varepsilon/k_{\rm B}T_{\rm c}}-1}
$$

Substituting in our form for $g(\varepsilon)$, we obtain

$$
n = \frac{3}{4\pi^2}\,\Gamma\big(\tfrac{9}{2}\big)\,\zeta\big(\tfrac{9}{2}\big)\,\bigg(\frac{k_{\rm B}T}{A}\bigg)^{9/2}\ ,
$$

and therefore

$$
T_{\rm c} = \frac{A}{k_{\rm B}}\,\bigg(\frac{4\pi^2 n}{3\,\Gamma\big(\frac{9}{2}\big)\,\zeta\big(\frac{9}{2}\big)}\bigg)^{2/9}
$$