PHYSICS 210A : STATISTICAL PHYSICS HW ASSIGNMENT #6 SOLUTIONS

(1) 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 $\mu = \varepsilon_0 - \frac{k_{\rm B}T}{g_0 N_0}$, 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

$$N_1 = \frac{\mathbf{g}_1}{e^{(\varepsilon_1 - \mu)/k_{\mathrm{B}}T} - 1} \approx \frac{\mathbf{g}_1 k_{\mathrm{B}}T}{\varepsilon_1 - \mu} \,,$$

assuming $\varepsilon_1 - \mu \ll k_{\rm B}T$. Now

$$\varepsilon_1 - \mu = (\varepsilon_0 - \mu) + (\varepsilon_1 - \varepsilon_0) = \frac{k_{\rm B}T}{g_0 N_0} + (\varepsilon_1 - \varepsilon_0) \; .$$

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.

(2) 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 $\Delta \rightarrow \infty$, 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 $\Delta \ll k_{\rm B}T_{\rm c}(n,\Delta = \infty)$, find analytically the leading order difference $T_{\rm c}(n,\Delta) - T_{\rm c}(n,\Delta = \infty)$.

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,

$$\begin{split} n &= \int_{-\infty}^{\infty} d\varepsilon \; \frac{g(\varepsilon)}{e^{(\varepsilon-\mu)/k_{\rm B}T} - 1} \\ &= {\rm Li}_{3/2} \big(e^{(\mu+\Delta)/k_{B}T} \big) \; \lambda_{T}^{-3} + {\rm Li}_{3/2} \big(e^{(\mu-\Delta)/k_{B}T} \big) \; \lambda_{T}^{-3} \; . \end{split}$$

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

$$n = n_0 + \zeta(3/2) \,\lambda_T^{-3} + \operatorname{Li}_{3/2} \left(e^{-2\Delta/k_{\mathrm{B}}T} \right) \lambda_T^{-3} \,.$$

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

$$n = \zeta(3/2) \,\lambda_{T_{\rm c}}^{-3} + {\rm Li}_{3/2} \big(e^{-2\Delta/k_{\rm B}T_{\rm c}} \big) \,\lambda_{T_{\rm c}}^{-3} \,.$$

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

$$k_{\rm B}T_{\rm c}^{\infty}(n) = \frac{2\pi\hbar^2}{m} \left(\frac{n}{\zeta(3/2)}\right)^{2/3}.$$

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

$$\zeta(3/2)\,\lambda_{T_{\rm c}}^{-3}\approx n-{\rm Li}_{3/2}\!\left(e^{-2\Delta/k_{\rm B}T_{\rm c}^\infty}\right)\lambda_{T_{\rm c}^\infty}^{-3}\;.$$

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

$$T_{\rm c}(n,\Delta) = T_{\rm c}^{\infty}(n) \left\{ 1 - \frac{3}{2} e^{-2\Delta/k_{\rm B}T_{\rm c}^{\infty}(n)} + \mathcal{O}\left(e^{-4\Delta/k_{\rm B}T_{\rm c}^{\infty}(n)}\right) \right\}.$$

(3) For an ideal Fermi gas in three dimensions,

- (a) Find an expression for the isothermal compressibility $\kappa_{T,N}$ as a function of the temperature *T* and fugacity *z*.
- (b) Find an expression for the adiabatic compressibility $\kappa_{S,N}$ as a function of the temperature *T* and fugacity *z*.
- (c) Find an expression for the ratio $C_{p,N}/C_{V,N}$ as a function of the temperature T and fugacity z.

Solution :

Recall

$$\begin{split} N &= V \!\!\!\!\int\limits_{-\infty}^{\infty} \!\!\!\!d\varepsilon \, g \, f \\ S &= -k_{\rm B} V \!\!\!\!\int\limits_{-\infty}^{\infty} \!\!\!\!d\varepsilon \, g \left\{ f \, \ln f + (1-f) \, \ln(1-f) \right\} \\ p &= -k_{\rm B} T \!\!\!\!\!\!\int\limits_{-\infty}^{\infty} \!\!\!\!d\varepsilon \, g \, \ln(1-f) \, , \end{split}$$

where $g = g(\varepsilon)$ and $f = f(\varepsilon - \mu)$ in the above expressions. Note further that the differential of the Fermi function is written in terms of dT and $d\mu$ as follows:

$$df = d\left(\frac{1}{e^{(\varepsilon-\mu)/k_{\rm B}T}+1}\right) = \left(-\frac{\partial f}{\partial \varepsilon}\right) \cdot \left\{(\varepsilon-\mu)\frac{dT}{T}+d\mu\right\}.$$

Thus, we have

$$V^{-1} dN = I_1 d \ln V + I_2 dT + I_3 d\mu$$
$$V^{-1} dS = J_1 d \ln V + J_2 dT + J_3 d\mu$$
$$dp = K_1 dT + K_2 d\mu ,$$

where

$$\begin{split} I_{1} &= \int_{-\infty}^{\infty} d\varepsilon \ g \ f \\ I_{2} &= \int_{-\infty}^{\infty} d\varepsilon \ g \left(-\frac{\partial f}{\partial \varepsilon} \right) \left(\frac{\varepsilon - \mu}{k_{\rm B} T} \right) \\ I_{3} &= \int_{-\infty}^{\infty} d\varepsilon \ g \left(-\frac{\partial f}{\partial \varepsilon} \right) \left(\frac{\varepsilon - \mu}{k_{\rm B} T} \right) \\ J_{3} &= k_{\rm B} \int_{-\infty}^{\infty} d\varepsilon \ g \left(-\frac{\partial f}{\partial \varepsilon} \right) \left(\frac{\varepsilon - \mu}{k_{\rm B} T} \right) \\ J_{3} &= k_{\rm B} \int_{-\infty}^{\infty} d\varepsilon \ g \left(-\frac{\partial f}{\partial \varepsilon} \right) \left(\frac{\varepsilon - \mu}{k_{\rm B} T} \right) \\ = k_{\rm B} I_{2} \end{split}$$

and

$$\begin{split} K_{1} &= -k_{\rm B} \int_{-\infty}^{\infty} d\varepsilon \; g \left\{ \ln(1-f) + \left(-\frac{\partial f}{\partial \varepsilon} \right) (\varepsilon - \mu) \right\} \\ K_{2} &= -k_{\rm B} T \int_{-\infty}^{\infty} d\varepsilon \; \frac{g}{1-f} \left(-\frac{\partial f}{\partial \varepsilon} \right) \end{split}$$

(a) Setting dT = dN = 0, we obtain $d\mu = -(I_1/I_3) d \ln V$, and therefore

$$\kappa_{T,N} = -\left(\frac{\partial \ln V}{\partial p}\right)_{T,N} = \frac{I_3}{I_1 K_2 - I_3 K_1} \,.$$

(b) Setting dN = dS = 0, we obtain

$$d\mu = \frac{I_1}{I_3} d\ln V + \frac{I_2}{I_3} dT = \frac{J_1}{J_3} d\ln V + \frac{J_2}{J_3} dT .$$

This can be used to express dT and $d\mu$ in terms of $d \ln V$ at fixed N and S. The final answer is quite involved and I won't reproduce it here. I regret asking this question!

(c) We set dN = 0 to write $d \ln V |_N$ in terms of dT and $d\mu$, and set dp = 0 to write $d\mu |_p = -(K_1/K_2) dT$. Thus, we can write both $d\mu$ and $d \ln V$ in terms of dT and compute $C_{p,N}$. For $C_{V,N}$, set $dN = d \ln V = 0$ to find $d\mu = -(I_2/I_3) dT$ and substitute into the equation for dS. Again the final result is somewhat tedious.

(4) At low energies, the conduction electron states in graphene can be described as fourfold degenerate fermions with dispersion $\varepsilon(\mathbf{k}) = \hbar v_{\rm F} |\mathbf{k}|$. Using the Sommerfeld expension,

- (a) Find the density of single particle states $g(\varepsilon)$.
- (b) Find the chemical potential $\mu(T, n)$ up to terms of order T^4 .

(c) Find the energy density $\mathcal{E}(T, n) = E/V$ up to terms of order T^4 .

Solution :

(a) The DOS per unit volume is

$$g(\varepsilon) = 4 \int \frac{d^2 k}{(2\pi)^2} \, \delta(\varepsilon - \hbar v_{\rm F} k) = \frac{2\varepsilon}{\pi (\hbar v_{\rm F})^2} \, .$$

(b) The Sommerfeld expansion is

$$\int_{-\infty}^{\infty} d\varepsilon f(\varepsilon - \mu) \phi(\varepsilon) = \int_{-\infty}^{\mu} d\varepsilon \phi(\varepsilon) + \frac{\pi^2}{6} (kT)^2 \phi'(\mu) + \frac{7\pi^4}{360} (k_{\rm B}T)^4 \phi'''(\mu) + \dots$$

For the particle density, set $\phi(\varepsilon) = g(\varepsilon)$, in which case

$$n = \frac{1}{\pi} \left(\frac{\mu}{\hbar v_{\rm F}}\right)^2 + \frac{\pi}{3} \left(\frac{k_{\rm B}T}{\hbar v_{\rm F}}\right)^2.$$

The expansion terminates after the $\mathcal{O}(T^2)$ term. Solving for μ ,

$$\mu(T,n) = \hbar v_{\rm F}(\pi n)^{1/2} \left[1 - \frac{\pi}{3n} \left(\frac{k_{\rm B}T}{\hbar v_{\rm F}} \right)^2 \right]^{1/2}$$
$$= \hbar v_{\rm F}(\pi n)^{1/2} \left\{ 1 - \frac{\pi}{6n} \left(\frac{k_{\rm B}T}{\hbar v_{\rm F}} \right)^2 - \frac{\pi^2}{72n^2} \left(\frac{k_{\rm B}T}{\hbar v_{\rm F}} \right)^4 + \dots \right\}$$

(c) For the energy density \mathcal{E} , we take $\phi(\varepsilon) = \varepsilon g(\varepsilon)$, whence

$$\mathcal{E}(T,n) = \frac{2\mu}{3\pi} \left[\left(\frac{\mu}{\hbar v_{\rm F}} \right)^2 + \left(\frac{\pi k_{\rm B} T}{\hbar v_{\rm F}} \right)^2 \right]$$
$$= \frac{2}{3} \sqrt{\pi} \hbar v_{\rm F} n^{3/2} \left\{ 1 + \frac{\pi}{2n} \left(\frac{k_{\rm B} T}{\hbar v_{\rm F}} \right)^2 - \frac{\pi^2}{8n^2} \left(\frac{k_{\rm B} T}{\hbar v_{\rm F}} \right)^4 + \dots \right\}$$