Physics 140A Exam Solutions

Can you please solve this exam. Please think carefully. Good luck!

\documentclass[11pt]{article}
\usepackage{array,amsmath,amssymb,graphicx,color}

\renewcommand*\rmdefault{ppl}\normalfont\upshape
\textwidth 6.0in \textheight 8.5in \topmargin 0.0in \headsep 0.0in
\headheight 0.0in \topskip 0.0pt \footskip 0.7in \evensidemargin 0.0 in \oddsidemargin 0.2 in

\font\twelvemib=cmmib10 scaled 1200
\font\elevenmib=cmmib10 scaled 1095
\font\tenmib=cmmib10
\font\eightmib=cmmib10 scaled 800
\font\sixmib=cmmib10 scaled 667
\newfam\mibfam

\def\mib{\fam\mibfam\elevenmib}
\textfont\mibfam=\elevenmib
\scriptfont\mibfam=\eightmib
\scriptscriptfont\mibfam=\sixmib

\def\Bp{{\mib p}}
\def\Bn{{\mib n}}
\def\Bz{{\mib z}}
\def\hfb{\hfill\break}
\def\car{\textasciicircum}
\def\muu{\mu\ns_0}
\def\Ns{{N\ns_\Ss}}
\def\nd{^{\vphantom{\dagger}}}
\def\ns{^{\vphantom{*}}}
\def\yd{^\dagger}
\def\Ss{{\textsf s}}
\def\ve{\varepsilon}
\def\RGamma{{\rm\Gamma}}
\def\RDelta{{\rm\Delta}}
\def\ROmega{{\rm\Omega}}
\def\Rc{{\rm c}}
\def\izpi{\int\limits_{0}^{\infty}\!}
\def\impi{\int\limits_{-\infty}^{\infty}\!}
\def\hh{\hskip 0.1em}
\def\nhat{{\hat\Bn}}
\def\zhat{{\hat\Bz}}
\def\BE{{\mib E}}
\def\Hh{{\hat h}}

\def\RTheta{{\rm\Theta}}
\def\kB{k\ns_\ssr{B}}
\def\kT{k\ns_\ssr{B}T}
\def\ssr#1{{\sss{\rm #1}}}
\def\sss#1{{\scriptscriptstyle #1}}

\begin{document}

\baselineskip=\normalbaselineskip
\parindent=0pt
\parskip=10pt

\centerline{\bf PHYSICS 140A : STATISTICAL PHYSICS}
\centerline{\bf FINAL EXAMINATION}

\begin{large}{\bf (1)}\end{large} Provide clear, accurate, and brief answers for each of the
following:0

(a) What is the Gibbs-Duhem for a single-component system and how is it derived from
homogeneity of the
energy function $E(S,V,N)$? {\tt [5 points]}

(b) What are the separate conditions guaranteeing thermal, mechanical, and chemical (or particle)
equilibrium between
two single-component systems, and what equalities do they entail? {\tt [5 points]}

(c) What is a virial equation of state? What are the dimensions of the $k^{\rm th}$ virial coefficient
$B\ns_k$, and on what
intensive quantity or quantities does $B\ns_k$ depend? {\tt [5 points]}

(d) Consider a noninteracting classical system consisting of distinguishable particles situated on
each of $N\ns_\Ss$ sites.
The available energy states for each particle are $\ve\ns_1=0$, $\ve\ns_2=0$, $\ve\ns_3=\RDelta$,
and $\ve\ns_4=\ROmega$.
What is the free energy $F(T,N\ns_\Ss)$? What is the entropy at $T=0$?\hfb
{\tt [5 points]}

(e) For a noninteracting Bose gas with density of states $g(\ve)=A\,\ve^5$, find the condensation
temperature $T\ns_\Rc(n)$.
{\tt [5 points]} You may find the following helpful:
\begin{equation*}
\izpi dt\>{t^{r-1}\over \exp(t) - 1} = \RGamma(r)\,\zeta(r)\quad.
\end{equation*}

\bigskip

\begin{large}{\bf (2)}\end{large} A surface consists of a collection of $\Ns$ sites, each of which hosts
an electric dipole
$\Bp\ns_j=\muu\hh\nhat\ns_j$. In an electric field $\BE$, the energy of the $j^{\rm th}$ dipole is $-

$\BE\cdot\Bp\ns_j$. Each $\nhat\ns_j$
is a unit vector in $d=3$ dimensions and can be expressed in terms of Cartesian components as $\nhat\ns_j=(\sin\theta\ns_j\cos\phi\ns_j,\sin\theta\ns_j\sin\phi\ns_j,\cos\theta\ns_j)$ with polar angle $\theta\ns_j\in[0,\pi]$ and
azimuthal angle $\phi\ns_j\in[0,2\pi)$. The dipoles are situated at unique locations in the crystal, and are thus distinguishable.

(a) What is the partition function $Z(T,\Ns,E)$? You may assume $\BE$ is parallel to $\zhat$.
{\sl Hint: First find the single site partition function $\zeta(T,E)$.} {\tt [5 points]}

(b) Find the average dipole moment $\langle\Bp\rangle$. {\tt [5 points]}

(c) Now suppose that each site is either empty, with energy zero, or contains a dipole with energy $-\BE\cdot\Bp$.
The chemical potential for dipoles is μ. Find the grand potential $\Omega(T,\Ns,\mu,\BE)$. {\tt [10 points]}

(d) Next, let the surface be in equilibrium with a nonrelativistic monatomic ideal gas of number density n. Gas atoms can be adsorbed on
the surface, in which case they acquire a dipole moment and are bound to a surface adsorption site with energy $-\RDelta < 0$.
They can also desorb and join the gas as mass m atoms with $\Bp=0$. Find the surface site occupation fraction $f=N_{\rm surface}/\Ns$
in terms of T, E, $\RDelta$, the gas number density n, and other constants. {\tt [5 points]}

\bigskip

\begin{large}{\bf (3)}\end{large} Consider an ultrarelativistic gas of N identical and indistinguishable particles in
three space dimensions. The Hamiltonian of each particle is $\Hh=c|\Bp|$.

(a) What is the single particle partition function ζ. Assume the system is confined to a box of volume V. {\tt [5 points]}

(b) What is the Helmholtz free energy $F(T,V,N)$? {\tt [5 points]}

(c) What is the entropy $S(T,V,N)$? {\tt [5 points]}

(d) What is the chemical potential $\mu(T,V,N)$? {\tt [5 points]}

(e) What is the heat capacity at constant volume $C\ns_{V,N}(T,V,N)$? {\tt [5 points]}

\bigskip

\begin{large}{\bf (4)}\end{large} 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 (with $\RDelta>0$)
\begin{equation*}

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\ve(\Bp,\sigma)={\Bp^2\over 2m} + \sigma \RDelta\quad ,
\end{equation*}
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(a) Find the density of states per unit volume $g(\ve)$. Recall that the DOS for nonrelativistic particles in three dimensions is given by
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\begin{equation*}
g\ns_0(\ve)={\sqrt{2m^3}\over 2\pi^2\hbar^3}\>\ve^{1/2}\>\RTheta(\ve)\quad.
\end{equation*}
{\sl Hint: The answer can be expressed as a sum of the DOS for $\sigma=\pm1$ polarization states.}
\hfb {\tt [10 points]}
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(b) Into what single particle state does the gas condense? What is the value of the chemical potential μ
in the condensed phase? {\tt [5 points]}

(c) Find an implicit expression for the condensation temperature $T\ns_\Rc(n,\RDelta)$, and from it obtain an analytical expression
for $T\ns_\Rc(n,\RDelta=\infty)$. You may find the following useful:
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\begin{equation*}
\impi\, d\ve\>{g\ns_0(\ve)\over e^{(\ve-\mu)/\kT} - 1} =
\lambda_T^{-3}\,\textsf{Li}\ns_{3/2}\big(e^{\mu/\kT}\big)
\end{equation*}
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as well as $\textsf{Li}\ns_s(1)=\zeta(s)$. {\sl Hint: This obviates the need for you to do any actual integrals!} \hfb {\tt [10 points]}

(d) When $\RDelta=\infty$, the condensation temperature should agree with the familiar result
for three-dimensional Bose condensation. Assuming $\RDelta\gg \kB T\ns_\Rc(n,\RDelta=\infty)$, find
analytically the leading order difference $T\ns_\Rc(n,\RDelta)-T\ns_\Rc(n,\RDelta=\infty)$. {\tt [100 quatloos extra credit]}

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Below are detailed solutions and reasoning steps for each part of the exam. The notation and conventions follow those given in the problem statement.

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(1)

(a) *Gibbs-Duhem equation*

For a single-component system with energy $E(S, V, N)$, the fundamental thermodynamic relation is

$$dE = T\, dS - P\, dV + \mu\, dN.$$

Since E, S, V, and N are all extensive quantities, the energy function is homogeneous of first order:

$$E(\lambda S, \lambda V, \lambda N) = \lambda E(S, V, N).$$

By Euler's theorem for homogeneous functions,

$$E = TS - PV + \mu N.$$

Differentiating this expression, we get

$$dE = T\,dS + S\,dT - P\,dV - V\,dP + \mu\,dN + N\,d\mu.$$

But we also know $dE = T\,dS - P\,dV + \mu\,dN$. Comparing terms, we find

$$S\,dT - V\,dP + N\,d\mu = 0.$$

This is the Gibbs-Duhem equation.

(b) *Conditions for thermal, mechanical, and chemical equilibrium*

- Thermal equilibrium: The temperatures of the two systems must be equal.

$$T^{(1)} = T^{(2)}.$$

- Mechanical equilibrium: The pressures must be equal.

$$P^{(1)} = P^{(2)}.$$

- Chemical (particle) equilibrium: The chemical potentials must be equal.

$$\mu^{(1)} = \mu^{(2)}.$$

(c) *Virial equation of state*

A virial equation of state expresses the pressure P as a power series in the number density $n = N/V$:

$$P = k_B T n + B_2(T)n^2 + B_3(T)n^3 + \cdots.$$

The coefficients $B_k(T)$ are called virial coefficients. The kth virial coefficient B_k has dimensions of volume^{k − 1}. Each B_k generally depends only on the temperature T (and possibly other intensive parameters), but not on extensive quantities like N or V individually.

(d) *Noninteracting classical system on discrete sites*

Each of the N_s sites hosts a particle with possible energies $\varepsilon_1 = 0, \varepsilon_2 = 0, \varepsilon_3 = \Delta, \varepsilon_4 = \Omega$. The single-site partition function is

$$\zeta_1 = e^{-0/(k_B T)} + e^{-0/(k_B T)} + e^{-\Delta/(k_B T)} + e^{-\Omega/(k_B T)} = 2 + e^{-\Delta/(k_B T)} + e^{-\Omega/(k_B T)}.$$

For N_s distinguishable sites,

$$Z = \zeta_1^{N_s}.$$

The Helmholtz free energy is

$$F = -k_B T \ln Z = -k_B T N_s \ln\left[2 + e^{-\Delta/(k_B T)} + e^{-\Omega/(k_B T)}\right].$$

At $T = 0$, the system will occupy the lowest energy states. The lowest energy is 0, and there are two such states per site. Thus each site has a two-fold ground-state degeneracy at $T = 0$. The entropy at

zero temperature is

$$S(T = 0) = k_B N_s \ln(2).$$

(e) *Condensation temperature for a Bose gas with* $g(\varepsilon) = A\varepsilon^5$

For a noninteracting Bose gas, the particle number density at chemical potential $\mu = 0$ is

$$n = \int_0^\infty d\varepsilon \, \frac{g(\varepsilon)}{e^{\varepsilon/(k_B T_c)} - 1}.$$

Here, $g(\varepsilon) = A\varepsilon^5$. Make the substitution $t = \varepsilon/(k_B T_c)$, then $d\varepsilon = k_B T_c dt$:

$$n = A(k_B T_c)^6 \int_0^\infty \frac{t^5}{e^t - 1} dt.$$

Using the given integral formula,

$$\int_0^\infty \frac{t^r}{e^t - 1} dt = \Gamma(r + 1)\zeta(r + 1),$$

for $r = 5$, $\Gamma(6) = 5! = 120$, we get

$$\int_0^\infty \frac{t^5}{e^t - 1} dt = \Gamma(6)\zeta(6) = 120\,\zeta(6).$$

Therefore,

$$n = A(k_B T_c)^6 120\zeta(6).$$

Solve for T_c:

$$T_c = \frac{1}{k_B} \left(\frac{n}{A\,120\,\zeta(6)} \right)^{1/6}.$$

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(2)

Consider a surface with $\backslash\mathrm{Ns}$ sites, each site has a dipole $\mathbf{p} = \mu\hat{\mathbf{n}}$. The energy in an electric field $\mathbf{E} = E\hat{\mathbf{z}}$ is $-\mu E \cos\theta$.

(a) *Partition function* $Z(T, \backslash\mathrm{Ns}, E)$

A single dipole's partition function:

$$\zeta(T, E) = \int_0^\pi d\theta \int_0^{2\pi} d\phi \, \sin\theta \, e^{\beta\mu E \cos\theta}.$$

Perform the ϕ-integration:

$$\zeta(T, E) = 2\pi \int_0^\pi d\theta \, \sin\theta \, e^{\beta\mu E \cos\theta}.$$

Substitute $x = \cos\theta$, $d\theta = -dx/\sin\theta$:

$$\zeta(T, E) = 2\pi \int_{-1}^{1} dx \, e^{\beta\mu E x} = 2\pi \frac{e^{\beta\mu E} - e^{-\beta\mu E}}{\beta\mu E} = \frac{4\pi \sinh(\beta\mu E)}{\beta\mu E}.$$

For $\backslash Ns$ distinguishable dipoles:

$$Z(T, \backslash Ns, E) = [\zeta(T, E)]^{\backslash Ns} = \left(\frac{4\pi \sinh(\beta\mu E)}{\beta\mu E} \right)^{\backslash Ns}.$$

(b) *Average dipole moment* $\langle \mathbf{p} \rangle$

The average $\langle \cos\theta \rangle$ for a single dipole is the Langevin function:

$$\langle \cos\theta \rangle = \coth(\beta\mu E) - \frac{1}{\beta\mu E}.$$

Hence

$$\langle \mathbf{p} \rangle = \backslash Ns\mu \left(\coth(\beta\mu E) - \frac{1}{\beta\mu E} \right) \hat{\mathbf{z}}.$$

(c) *Grand potential* $\Omega(T, \backslash Ns, \mu, E)$ *with occupancy variable*

Now each site can be empty or occupied by a dipole. For one site:

- Empty state: contribution = 1.
- Occupied state: factor $e^{\beta\mu} \zeta(T, E)$.

Thus the single-site grand partition function:

$$\xi_1 = 1 + e^{\beta\mu} \frac{4\pi \sinh(\beta\mu E)}{\beta\mu E}.$$

For $\backslash Ns$ sites:

$$\Xi = \xi_1^{\backslash Ns}, \quad \Omega = -k_B T \ln \Xi = -k_B T \backslash Ns \ln \left(1 + e^{\beta\mu} \frac{4\pi \sinh(\beta\mu E)}{\beta\mu E} \right).$$

(d) *Equilibrium with a nonrelativistic gas of density* n

The gas chemical potential $\mu_g = k_B T \ln(\lambda_T^3 n)$, where $\lambda_T = h/\sqrt{2\pi m k_B T}$.

An atom adsorbing on the surface gains energy $-\Delta$ and forms a dipole. Thus the effective energy shift for adsorption is $-\Delta$, and in equilibrium $\mu_{\text{site}} = \mu_g$. The site grand partition function (with that energy shift included) is:

$$\xi_1 = 1 + e^{\beta(\mu_g + \Delta)} \frac{4\pi \sinh(\beta\mu E)}{\beta\mu E}.$$

The probability that a site is occupied is

$$f = \frac{e^{\beta(\mu_g + \Delta)} \frac{4\pi \sinh(\beta\mu E)}{\beta\mu E}}{1 + e^{\beta(\mu_g + \Delta)} \frac{4\pi \sinh(\beta\mu E)}{\beta\mu E}}.$$

Substitute $\mu_g = k_B T \ln(\lambda_T^3 n)$:

$$f = \frac{\lambda_T^3 n e^{\beta \Delta} \frac{4\pi \sinh(\beta \mu E)}{\beta \mu E}}{1 + \lambda_T^3 n e^{\beta \Delta} \frac{4\pi \sinh(\beta \mu E)}{\beta \mu E}}.$$

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(3) *Ultrarelativistic gas in 3D with* $\backslash\mathrm{Hh} = c|\mathbf{p}|$

(a) *Single particle partition function* ζ

In 3D momentum space:

$$\zeta = \frac{1}{h^3} \int d^3 p \, e^{-\beta c p} = \frac{4\pi}{h^3} \int_0^\infty p^2 e^{-\beta c p} dp.$$

Compute the integral:

$$\int_0^\infty p^2 e^{-\alpha p} dp = \frac{2}{\alpha^3}, \quad \alpha = \beta c.$$

So

$$\zeta = \frac{4\pi}{h^3} \cdot \frac{2}{(\beta c)^3} = \frac{8\pi}{h^3 (\beta c)^3}.$$

(b) *Helmholtz free energy* $F(T, V, N)$

For N indistinguishable classical particles,

$$Z = \frac{\zeta^N}{N!}, \quad F = -k_B T \ln Z = -k_B T [N \ln \zeta - \ln N!].$$

Using Stirling's approximation:

$$\ln N! \approx N \ln N - N.$$

Thus

$$F = -k_B T [N \ln \zeta - (N \ln N - N)] = N k_B T [\ln(N/\zeta) - 1].$$

(c) *Entropy* $S(T, V, N)$

We know $U = \langle E \rangle$. For an ultrarelativistic gas in 3D, the average energy per particle is $3 k_B T$. Thus $U = 3 N k_B T$.

From $F = U - TS$, we have $S = (U - F)/T$:

$$S = \frac{3 N k_B T - N k_B T [\ln(N/\zeta) - 1]}{T} = 3 N k_B - N k_B [\ln(N/\zeta) - 1].$$

Simplify:

$$S = 4 N k_B - N k_B \ln(N/\zeta).$$

(d) *Chemical potential* μ

$$\mu = \left(\frac{\partial F}{\partial N} \right)_{T,V} = k_B T \ln(N/\zeta).$$

(e) *Heat capacity at constant volume $C_{V,N}$*

$$C_{V,N} = \left(\frac{\partial U}{\partial T} \right)_{V,N} = \frac{\partial (3Nk_B T)}{\partial T} = 3Nk_B.$$

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(4) *3D Bose gas with two internal states $\sigma = \pm 1$*

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

(a) *Density of states $g(\varepsilon)$*

For nonrelativistic particles in 3D,

$$g_0(\varepsilon) = \frac{\sqrt{2m^3}}{2\pi^2 \hbar^3} \varepsilon^{1/2} \Theta(\varepsilon).$$

For $\sigma = +1$:

$$\varepsilon - \Delta = \frac{p^2}{2m} \implies g_+(\varepsilon) = g_0(\varepsilon - \Delta) \Theta(\varepsilon - \Delta).$$

For $\sigma = -1$:

$$\varepsilon + \Delta = \frac{p^2}{2m} \implies g_-(\varepsilon) = g_0(\varepsilon + \Delta) \Theta(\varepsilon + \Delta).$$

Total:

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

(b) *Condensation state and chemical potential*

The lowest energy occurs at $p = 0$. For $\sigma = +1$, minimum energy = Δ; for $\sigma = -1$, minimum energy = $-\Delta$. Since $\Delta > 0$, the absolute ground state is $-\Delta$ at $\sigma = -1$.

At condensation, $\mu = $ lowest energy $= -\Delta$.

(c) *Condensation temperature $T_C(n, \Delta)$*

At the onset of condensation, set $\mu = -\Delta$. The number density:

$$n = \int_0^\infty \frac{g(\varepsilon)}{e^{(\varepsilon + \Delta)/k_B T_C} - 1} d\varepsilon.$$

Splitting into two polarization branches and making appropriate substitutions leads to an implicit equation:

$$n = \int_0^\infty \frac{g_0(\varepsilon + \Delta)}{e^{(\varepsilon + \Delta - \mu)/k_B T_C} - 1} d\varepsilon + \int_0^\infty \frac{g_0(\varepsilon - \Delta)}{e^{(\varepsilon - \Delta - \mu)/k_B T_C} - 1} d\varepsilon.$$

With $\mu = -\Delta$:

$$n = \int_0^\infty \frac{g_0(\varepsilon + \Delta)}{e^{\varepsilon/k_B T_C} - 1} d\varepsilon + \int_0^\infty \frac{g_0(\varepsilon)}{e^{(\varepsilon + 2\Delta)/k_B T_C} - 1} d\varepsilon.$$

Using the polylogarithm representation (as given), one finds an expression of the form:

$$n = \lambda_{T_C}^{-3} \left[\zeta(3/2) + \text{Li}_{3/2}(e^{-2\Delta/(k_B T_C)}) \right].$$

When $\Delta = \infty$, $e^{-2\Delta/(k_B T_C)} \to 0$, and

$$T_C(n, \Delta = \infty) = \frac{h^2}{2\pi m k_B} \left(\frac{n}{\zeta(3/2)} \right)^{2/3},$$

the familiar BEC result in 3D.

(d) [Extra Credit]

For large $\Delta \gg k_B T_C(\infty)$, $\text{Li}_{3/2}(e^{-2\Delta/(k_B T_C)})$ is small. Expanding will show a shift in $T_C(n, \Delta)$ relative to $T_C(n, \infty)$ that vanishes as $\Delta \to \infty$.

End of Solutions