STATISTICAL PHYSICS 215A

Final Exam – Spring 2019

Monday 10 June 2019 from 3pm to 6pm in room PAB-2-434

- **Print your name on every pages used, including this one;**
- Make clear which question you are answering on each page;

- No books, notes, computers, or calculators are allowed during the exam;
- Please turn off cell-phones, iPhones, iPods, iPads, Kindles, and other electronic devices.

- Please write clearly; present your arguments and calculations clearly;
- All four questions below are independent from one another.

Grades

Q1.

Q2.

Q3.

Q4.

Total /65

QUESTION 1 [16 points]

A gas of mono-atomic particles of mass m that deviates slightly from ideal behavior obeys the following equation of state,

$$PV = NkT - a\frac{N^2}{V}$$

where P is the pressure, T the temperature, N the number of particles, and a is a constant.

a) Deduce the dependence of the partition function Z on the volume V.

b) Use your knowledge of the ideal gas to obtain the fully normalized partition function, including the proper quantum normalization for phase space and indistinguishability.

c) Compute the internal energy E.

d) Compute the specific heat at constant pressure C_P in terms of T, V, N, using the results obtained in b) and c).

QUESTION 2 [18 points]

Consider an ideal gas of spin-1 bosons of mass $m > 0$ in the presence of a constant uniform magnetic field B in the z-direction, governed by the Hamiltonian,

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

where $\kappa = e\hbar/mc$, we assume $\kappa, B > 0$, and the spin operator S_z can take the values $(-1, 0, +1)$.

a) In the grand canonical ensemble for chemical potential μ and temperature T, obtain the average occupation numbers $n_-(\mathbf{p})$, $n_0(\mathbf{p})$, and $n_+(\mathbf{p})$ of one-particle states with momentum $\mathbf{p}$ for the three possible spin states.

b) Calculate the corresponding average total numbers of bosons N_-, N_0, and N_+ in each spin state in terms of the function,

$$g_\nu(z) = \frac{1}{\Gamma(\nu)} \int_0^\infty dx \, \frac{x^{\nu-1}}{z^{-1}\, e^x - 1} = \sum_{n=1}^\infty \frac{z^n}{n^\nu}$$

c) Obtain the total magnetization $M = \kappa(N_+ - N_-)$ and, by expanding M for small B, obtain the magnetic susceptibility $\chi(T, \mu)$ at zero magnetic field.

d) Find the critical temperature T_c at which Bose-Einstein condensation occurs as a function of the total particle density $n = (N_- + N_0 + N_+)/V$ where V is the volume.

e) What is the chemical potential μ for $T < T_c$? Which one-particle state has macroscopic occupation umber ?

f) Using the results from e), find the spontaneous magnetization for $B = 0$.

QUESTION 3 [13 points]

A crystal consists of N atoms. When n atoms in a perfect crystal (where $1 \ll n \ll N$) are displaced from lattice sites inside the crystal to lattice sites on the surface, the crystal becomes imperfect, and has defects. Let $w > 0$ be the energy necessary to displace an atom from the inside to the surface. Assuming equilibrium at temperature T (with $kT \ll w$), determine an approximate formula for the number of displaced sites n in terms of N, w, and T. Neglect any effect due to the change in volume of the crystal.

QUESTION 4 [18 points]

We propose to evaluate the electric current density of electrons which is produced by the photo-electric effect due to incoming mono-chromatic light with angular frequency ω. The photo-electric effect in a metal occurs when a conduction electron in the metal absorbs a photon and acquires enough additional energy to escape from the surface. Assume that the surface of the metal is along the xy-plane and that the electrons are emitted along the z-direction perpendicular to the surface without affecting the momenta in the xy directions. We denote the potential energy of the electrons in the interior of the metal by $-W$, with $W > 0$ and the potential energy outside of the metal being zero. The vertical kinetic energy of the electron is by $\varepsilon_z = p_z^2/2m$.

a) Give a formula for the minimum value of ε_z needed for the electron to escape the metal upon absorbing a photon of energy $\hbar\omega$.

b) Derive an integral formula for the electric current density J_z in the z-direction in terms of the variables $W, \hbar\omega$, the temperature T and the chemical potential μ for the electrons.

c) Integrate out the momenta in the xy directions and show that the current is given by the following integral representation,

$$J_z = A(kT)^2 \Phi\left(\frac{\hbar(\omega - \omega_0)}{kT}\right)$$

where the function $\Phi(\delta)$ is given by,

$$\Phi(\delta) = \int_0^\infty dx \ln(1 + e^{\delta - x})$$

d) Determine A and ω_0 in terms of W, μ and various fundamental constants of Nature.

e) Determine the leading behavior of the integral $\Phi(\delta)$ for $\delta \to +\infty$ and deduce the current density J_z for $\omega \gg \omega_0$.

f) Determine the leading behavior of the integral $\Phi(\delta)$ for $\delta \to -\infty$ and deduce the current density J_z for $\omega \ll \omega_0$.

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QUESTION 1 - solution [16 points]

a) The partition function Z of the canonical ensemble is related to the Helmholtz free energy F by $F = -kT \ln Z$. Using the expression for the pressure P in terms of F, and equating it with the expression for P from the equation of state, we find,

$$P = -\frac{\partial F}{\partial V}\Big|_{T,N} = kT\,\frac{\partial \ln Z}{\partial V}\Big|_{T,N} = \frac{NkT}{V} - a\frac{N^2}{V^2}$$

Dividing through by kT and integrating to get Z, we find,

$$\ln Z = N \ln V + a\frac{N^2}{VkT} + f(T,N)$$

for some function f which depends only on T and N.

b) The partition function for the mono-atomic ideal gas is given by,

$$Z_{a=0} = \frac{Z_1^N}{N!} \qquad Z_1 = \int \frac{V\,d^3p}{(2\pi\hbar)^3}\, e^{-\beta p^2/2m} = \frac{V}{\lambda^3} \qquad \lambda^2 = \frac{2\pi\hbar^2}{mkT}$$

and since f is independent of V, this determines f by taking the large V limit, for T and N fixed, and we find the properly normalized and manifestly extensive expression,

$$\ln Z = N \ln\frac{V}{N} + N - 3N\ln\lambda + a\frac{N^2}{VkT}$$

c) The internal energy is given by,

$$E = -\frac{\partial \ln Z}{\partial \beta}\Big|_{V,N} = \frac{3}{2}NkT - a\frac{N^2}{V}$$

d) To compute the specific heat at constant pressure, we change variables and use the enthalpy $H = E + PV$ with $dH = TdS + VdP + \mu dN$. Thus, the specific heat C_P is then given by,

$$C_P = T\frac{\partial S}{\partial T}\Big|_{P,N} = \frac{\partial H}{\partial T}\Big|_{P,N} = \frac{\partial}{\partial T}\left(\frac{5}{2}NkT - 2a\frac{N^2}{V}\right)\Big|_{P,N} = \frac{5}{2}Nk + 2a\frac{N^2}{V^2}\frac{\partial V}{\partial T}\Big|_{P,N}$$

The derivative of V with respect to T keeping P,N fixed is obtained by differentiating the equation of state, and we find,

$$\left(P - a\frac{N^2}{V^2}\right)\frac{\partial V}{\partial T}\Big|_{P,N} = \left(\frac{NkT}{V} - 2a\frac{N^2}{V^2}\right)\frac{\partial V}{\partial T}\Big|_{P,N} = Nk$$

so that the final result is given by,

$$C_P = Nk\left(\frac{5}{2} + \frac{2aN}{kTV - 2aN}\right)$$

QUESTION 2 - solution [18 points]

a) The occupation numbers with $s = 0, \pm 1$ are given by,

$$n_s(\mathbf{p}) = \frac{1}{e^{\beta(\mathbf{p}^2/2m - s\kappa B - \mu)} - 1}$$

b) The corresponding numbers of particles are given by,

$$N_s = \int \frac{V d^3p}{(2\pi\hbar)^3} \frac{1}{e^{\beta(\mathbf{p}^2/2m - s\kappa B - \mu)} - 1}$$

or in terms of the functions g_ν,

$$N_s = \frac{V}{\lambda^3} g_{\frac{3}{2}}(e^{\beta(\mu + s\kappa B)}) \qquad\qquad \lambda^2 = \frac{2\pi\hbar^2}{mkT}$$

c) The magnetization is given by,

$$M = \frac{\kappa V}{\lambda^3} \left(g_{\frac{3}{2}}(e^{\beta(\mu+\kappa B)}) - g_{\frac{3}{2}}(e^{\beta(\mu-\kappa B)}) \right)$$

Expanding for small B to linear order, we find,

$$M = \frac{2\kappa^2 BV}{\lambda^3 kT} z g'_{\frac{3}{2}}(z) + \mathcal{O}(B^3) \qquad\qquad z = e^{\beta\mu}$$

Using $z g'_{\frac{3}{2}}(z) = g_{\frac{1}{2}}(z)$, and extracting the susceptibility at zero magnetic field, we find,

$$\chi(T, \mu) = \frac{2\kappa^2 V}{\lambda^3 kT} g_{\frac{1}{2}}(z) + \mathcal{O}(B^2)$$

d) Bose-Einstein condensation occurs at $z = 1$ where the ground state will have macroscopic occupation number. In terms of the total number of particles at $B = 0$, the relation is given by,

$$\rho = \frac{3}{\lambda^3} g_{\frac{3}{2}}(1) = \frac{3}{\lambda^3} \zeta(\frac{3}{2}) \qquad\qquad T_c(B = 0) = \frac{2\pi\hbar^2}{mk} \left(\frac{\rho}{2\zeta(\frac{3}{2})} \right)^{\frac{2}{3}}$$

e) For non-zero B, the chemical potential must obey $s\kappa B + \mu \leq 0$ for $s = 0, \pm 1$. Assuming that $\kappa B > 0$, this means $\mu \leq -\kappa B$, and at Bose-Einstein condensation point we will have

$$\mu = -\kappa B$$

The state $s = +1$ and $\mathbf{p} = 0$ is the one that will have macroscopic occupation number.

f) Below the critical temperature, the number of states above the ground state is given by $3V\zeta(\frac{3}{2})\lambda^{-3}$. For small $\kappa B > 0$ the number of condensed particles in the ground state is solely due to the state $s = +1$, so that the total magnetization as $B \to 0$ is given by

$$M = \kappa \left(N - \frac{3V}{\lambda^3} \zeta(\frac{3}{2}) \right) = \kappa N \left(1 - \left(\frac{T}{T_c} \right)^{\frac{3}{2}} \right)$$

where N is the total number of particles in the system.

QUESTION 3 - solution [13 points]

With n atoms displaced out of N atoms in the original perfect crustal, the number of accessible micro-states for $1 \ll n \ll N$ is given by $N!/(n!\,(N-n)!)$, so that the entropy is given by,

$$S(n) = k \ln \frac{N!}{n!\,(N-n)!} \approx k\Big(N \ln N - n \ln n - (N-n)\ln(N-n)\Big)$$

where we have used Stirling's formula to approximate the factorials. The internal energy of a state with n displaced atoms is nw, so that the free energy of the system is given by,

$$F = E - TS = nw - kT\Big(N \ln N - n \ln n - (N-n)\ln(N-n)\Big)$$

Extremizing in n, keeping N, T, and w fixed, we find,

$$0 = \frac{\partial F}{\partial n}\Big|_{T,N} = w - kT \ln \frac{N-n}{n}$$

so that we have,

$$n \approx N\, e^{-w/kT}$$

for $w \ll kT$.

QUESTION 4 - solution [18 points]

a) To escape from the metal, an electron must overcome the potential energy barrier W, as well as the chemical potential barrier μ. (Pahtria does not quite do this correctly and omits the chemical potential contribution; the correct treatment is in Kubo's book. A few students correctly included the chemical; for the others, I have subtracted only one point.) Therefore the energy ε_z must satisfy,

$$\varepsilon_z > W + \mu - \hbar\omega$$

b) The electric current density is given by the velocity of one electron, p_z/m times its electric charge e (taken here to be negative), times the number density of electrons, integrated over the allowed values of the momentum p_z, namely $p_z > p_0$ with $p_0 = \sqrt{2m(W + \mu - \hbar\omega)}$,

$$J_z = \frac{2e}{m} \int_{p_z > p_0}^{\infty} dp_z \int_{\mathbf{R}^2} \frac{dp_x dp_y}{(2\pi\hbar)^3} \frac{p_z}{e^{\beta(\mathbf{p}^2/2m - \mu)} + 1}$$

The overall factor of 2 is to account for the two spin states of the electron. Note that since we compute the current density, there is no factor of the volume of space.

c) Carrying out the integral over p_x and p_y by passing to polar coordinates and using rotational symmetry of the integrand, we find,

$$\int_{\mathbf{R}^2} \frac{dp_x dp_y}{(2\pi\hbar)^3} \frac{1}{e^{\beta(\mathbf{p}^2/2m - \mu)} + 1} = \frac{2\pi m k T}{(2\pi\hbar)^3} \ln\Big(1 + e^{-\beta(p_z^2/2m - \mu)}\Big)$$

Substituting this result into the expression for the current,

$$J_z = \frac{4\pi ekT}{(2\pi\hbar)^3} \int_{p_z > p_0}^{\infty} dp_z\, p_z \,\ln\left(1 + e^{-\beta(p_z^2/2m - \mu)}\right)$$

Changing variables from p_z to x with $2mkTx = p_z^2 - p_0^2$, we obtain,

$$J_z = \frac{4\pi em(kT)^2}{(2\pi\hbar)^3} \int_0^{\infty} dx\, \ln\left(1 + e^{-x+\delta}\right)$$

d) The above expression is exactly of the form announced with $W = \hbar\omega_0$ and,

$$\delta = \beta\left(\mu - \frac{p_0^2}{2m}\right) = \frac{\hbar(\omega - \omega_0)}{kT} \qquad\qquad A = \frac{4\pi em}{(2\pi\hbar)^3}$$

e) For $\delta \to \infty$, split the integral at $x = \delta$,

$$\Phi(\delta) = \int_0^{\delta} dx \ln\left(1 + e^{\delta - x}\right) + \int_{\delta}^{\infty} dx \ln\left(1 + e^{\delta - x}\right)$$

The second integral converges to a number independent of δ. In the first integral, the argument of the log is dominated by the second term, so that the log is approximately $\delta - x$, which upon integration produces,

$$\Phi(\delta) \approx \frac{1}{2}\delta^2$$

and thus

$$J_z \approx \frac{em}{4\pi^2\hbar}(\omega - \omega_0)^2 \qquad\qquad \omega \gg \omega_0$$

This result makes physical sense since the current density is independent of temperature for large incoming frequency.

f) For $\delta \to -\infty$, the exponential part of the argument of the log is small and the log may be approximated by the exponential alone,

$$\Phi(\delta) \approx \int_0^{\infty} e^{\delta - x} = e^{\delta}$$

Hence the current density is given by,

$$J_z \approx \frac{4\pi em(kT)^2}{(2\pi\hbar)^3} \exp\left\{\frac{\hbar(\omega - \omega_0)}{kT}\right\}$$

This also makes physical sense: the current density is exponentially suppressed by the gap $W - \hbar\omega \gg kT$.