Physics 607 Exam 2

Please be well-organized, and show all significant steps clearly in all problems.

You are graded on your work, so please do not just write down answers with no explanation!

Do all your work on the blank sheets provided, writing your name clearly. (You may keep this exam.)

The variables have their usual meanings: $E =$ energy, $S =$ entropy, $V =$ volume, $N =$ number of particles, $T =$ temperature, $P =$ pressure, $\mu =$ chemical potential, $B =$ applied magnetic field, $C_V =$ heat capacity at constant volume, $C_P =$ heat capacity at constant pressure, $F =$ Helmholtz free energy, $G =$ Gibbs free energy, $k =$ Boltzmann constant, $h =$ Planck constant. Also, $\langle \cdots \rangle$ represents an average.

$$\int_{-\infty}^{\infty} e^{-x^2} dx = \sqrt{\pi} \quad , \quad \int_{-\infty}^{\infty} x^2 e^{-x^2} dx = \frac{1}{2}\sqrt{\pi} \quad , \quad \int_0^{\infty} x^n e^{-x^2} dx = \frac{1}{2}\Gamma\left(\frac{n+1}{2}\right)$$

$$\Gamma\left(\frac{1}{2}\right) = \sqrt{\pi} \quad , \quad \Gamma(1) = 1 \quad , \quad \Gamma(z+1) = z\Gamma(z) \quad , \quad \ln N! \approx N \ln N - N \quad , \quad e^x = 1 + x + \frac{x^2}{2} + \ldots$$

$$E = TS - PV + \mu N \quad , \quad E = kT^2 \frac{\partial}{\partial T} \ln Z \quad , \quad F = -kT \ln Z \quad , \quad \left\langle x_i \frac{\partial H}{\partial x_j} \right\rangle = \delta_{ij} kT \quad , \quad \dot{p}_i = -\frac{\partial H}{\partial q_i} \quad , \quad \dot{q}_i = \frac{\partial H}{\partial p_i}$$

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1. The easiest way to do this problem is to use the equipartition theorem.

A classical system of noninteracting diatomic molecules is enclosed in a box of volume V at temperature T. The Hamiltonian of a single molecule is

$$H\left(\vec{r}_1,\vec{r}_2,\vec{p}_1,\vec{p}_2\right)=\frac{1}{2m}\left(\vec{p}_1^{\,2}+\vec{p}_2^{\,2}\right)+\frac{1}{2}K\left|\vec{r}_2-\vec{r}_1\right|^2$$

which can be transformed to center of mass coordinates $\vec{R}$ and $\vec{P}$ and relative coordinates (r,θ,ϕ) and $\left(p,p_\theta,p_\phi\right)$, becoming

$$H\left(\vec{r}_1,\vec{r}_2,\vec{p}_1,\vec{p}_2\right)=\frac{\vec{P}^2}{2M}+\frac{p^2}{2\mu}+\frac{p_\theta^2}{2I}+\frac{p_\phi^2}{2I\sin^2\theta}+\frac{1}{2}Kr^2$$

where M is the total mass, μ is the usual reduced mass, and $I=\mu r^2$.

(a) (8) First let us make the approximation that the moment of inertia I is constant.

In this approximation, calculate $\left\langle r^2\right\rangle$ as a function of T.

(b) (15) Now let us relax this approximation, so that the Hamiltonian includes the dependence of the moment of inertia on r in our classical Hamiltonian

$$H=\frac{\vec{P}^2}{2M}+\frac{p^2}{2\mu}+\frac{p_\theta^2}{2\mu r^2}+\frac{p_\phi^2}{2\mu r^2\sin^2\theta}+\frac{1}{2}Kr^2 \quad .$$

For this full Hamiltonian, calculate $\left\langle r^2\right\rangle$ as a function of T.

[In a quantum description there is a single vibrational coordinate, with the coupling between rotations and vibrations treated as a perturbation, along with anharmonicity.]

2. Recall that a Debye solid has a maximum vibrational angular frequency ω_D which is determined by the fact that there are $3N$ vibrational modes with N atoms. Assume two transverse modes with $\omega = v_t k$ and one longitudinal mode with $\omega = v_\ell k$, where $p = \hbar k$ is the (crystal) momentum and k is the wavenumber.

(a) (8) Using the fact that the density of states in momentum space is given by

$$\rho(p)dp = \frac{4\pi p^2 dp}{h^3 / V}$$

calculate the total density of states $\rho(\omega)$ for all three modes in terms of $\bar{v}$, where

$$\frac{3}{\bar{v}^3} \equiv \frac{2}{v_t^3} + \frac{1}{v_\ell^3} \quad .$$

(b) (8) Show that

$$\omega_D = \left(C \frac{N}{V} \right)^{1/3} \bar{v}$$

where you will determine the constant C.

(b) (9) Show that the zero-point energy of a Debye solid is equal to constant $\times\ N k_B \Theta_D$, where you will determine this constant. Here $\Theta_D = \hbar \omega_D / k_B$ is the Debye temperature and the Boltzmann constant is called k_B to avoid confusion.

3. Let us calculate the speed of sound u in an ideal quantum gas of fermions at $T = 0$ using

$$u^2 = \left(\frac{\partial P}{\partial \rho}\right)_{T=0}$$

where $\rho = mn$, m is the mass of one particle, and $n = \frac{N}{V}$ is the number density. (See the bottom of this page for the general expression for u.) These are nonrelativistic spin 1/2 fermions in 3 dimensions, with energy $\varepsilon = \frac{p^2}{2m}$.

(a) (4) Using the fact that the density of states in momentum space is given by

$$\rho(p)dp = \frac{4\pi p^2 dp}{h^3 / V}$$

calculate the value of the Fermi momentum p_F and the Fermi energy $\varepsilon_F = \frac{p_F^2}{2m}$ (in terms of the various constants). You should find that $p_F \propto n^{1/3}$, where you will determine the proportionality constant.

(b) (4) Again using this density of states, and the result for p_F, show that the energy of the system is given by

$$\frac{E}{V} = \text{ constant } \times \ n^{5/3}$$

while at the same time determining the constant.

(c) (4) For a nonrelativistic ideal gas, recall that $P = \frac{2}{3}\frac{E}{V}$. Calculate u at $T = 0$, giving your answer in terms of n and m .

(d) (4) Show that $u = \text{constant} \times u_F$, while at the same time obtaining the constant. Here u_F is the Fermi velocity: $\varepsilon_F = \frac{1}{2} m u_F^2$.

(e) (4) Using the standard expression for dE in terms of dS, dV, and dN, and the Euler relation for E in terms of TS, PV, and μN, obtain the Gibbs-Duhem relation involving $s\,dT$, $v\,dP$, and $d\mu$. Here $s = \frac{S}{N}$ and $v = \frac{V}{N}$.

(f) (4) Use the Gibbs-Duhem relation to obtain the relation between $\left(\frac{\partial P}{\partial n}\right)_T$ and $\left(\frac{\partial \mu}{\partial n}\right)_T$. Then obtain the relation between $\left(\frac{\partial P}{\partial \rho}\right)_T$ and $\left(\frac{\partial \mu}{\partial n}\right)_T$.

(g) (4) Finally, using the above relation and the fact that $\mu = \varepsilon_F$ at $T = 0$, again calculate u at $T = 0$, giving your answer in terms of n and m . Do you get the same answer as in Part (c)?

$u = \sqrt{\frac{1}{\rho \kappa_S}}$, $\kappa_S \equiv -\frac{1}{V}\left(\frac{\partial V}{\partial P}\right)_S$ = adiabatic compressibility , with $T = 0$ the same as $S = 0$.

4. Consider an ideal quantum gas of spinless bosons in D dimensions, with a relation between energy and momentum of the form $\varepsilon = ap^s$. We wish to determine the relation between D and s if Bose-Einstein condensation is to occur. (You can check your answer with what you know about a nonrelativistic system, with $s = 2$, in 2 and 3 dimensions. We are extending this to an ultrarelativistic system, with $s = 1$.)

Recall that the density of states in momentum space is given by

$$\rho(p)dp = A\,p^{D-1}dp \quad , \quad A = \frac{2\pi^{D/2}}{\Gamma(D/2)} \cdot \frac{1}{h^D/V}$$

where V is the D-dimensional volume in which the particles are confined.

(a) (4) At temperature T, write down the equation for the number of particles N in term of (i) the number of particles $N_0(T)$ in the state with $p = 0$ and (ii) an integral over p (i.e., over all the excited states with $p > 0$). Recall that

$$\langle n(\varepsilon) \rangle = \frac{\lambda}{e^{\varepsilon/kT} - \lambda} \quad , \quad \lambda = e^{\mu/kT} \; .$$

(b) (4) Derive the value of the chemical potential μ below the transition temperature if Bose-Einstein condensation is to occur – i.e., if the ground single-particle state is to contain an infinite number of particles – in the limit $N \to \infty$. (Please be clear in your argument.)

(c) (4) Assuming the value of the chemical potential μ obtained in Part (b), rewrite the integral of Part (a) as an integral over ε.

(d) (4) Using the result of part (c), obtain an equation of the form

$$N = \text{constant} \times T^{\alpha} + N_0$$

while at the same time obtaining the constant prefactor and the other constant α, in terms of A, D, s, etc.

(e) (4) Obtain the condition on D and s for Bose-Einstein condensation to be required.

(f) (4) For those cases where Bose-Einstein condensation does occur at some temperature $T_c \neq 0$, obtain $\frac{N_0}{N}$ as a function of $\frac{T}{T_c}$ for $T \leq T_c$.