8.333: Statistical Mechanics I Problem Set # 6 Due: 12/6/13 @ mid-night[†] † According to MIT regulations, no problem set can have a due date later than 12/6/13, and I have extended the due date to the last possible minute! However, you can be (and will be!) examined on material that is covered in December. The optional problems are part of this material; credit for them can be used to boost your overall homework grade.

Ideal Quantum Gases

1. Numerical estimates: The following table provides typical values for the Fermi energy and Fermi temperature for (i) Electrons in a typical metal; (ii) Nucleons in a heavy nucleus; and (iii) He³ atoms in liquid He³ (atomic volume = 46.2\AA^3 per atom).

	$n(1/\mathrm{m}^3)$	$m({ m Kg})$	$\varepsilon_F(\mathrm{eV})$	$T_F(\mathbf{K})$
electron	10^{29}	9×10^{-31}	4.4	$5 imes 10^4$
nucleons	10^{44}	1.6×10^{-27}	$1.0 imes 10^8$	1.1×10^{12}
liquid He^3	2.6×10^{28}	4.6×10^{-27}	$\times 10^{-3}$	10^{1}

(a) Estimate the ratio of the electron and phonon heat capacities at room temperature for a typical metal.

(b) Compare the thermal wavelength of a neutron at room temperature to the minimum wavelength of a phonon in a typical crystal.

(c) Estimate the degeneracy discriminant, $n\lambda^3$, for hydrogen, helium, and oxygen gases at room temperature and pressure. At what temperatures do quantum mechanical effects become important for these gases?

(d) Experiments on He⁴ indicate that at temperatures below 1K, the heat capacity is given by $C_V = 20.4T^3 J K g^{-1} K^{-1}$. Find the low energy excitation spectrum, $\mathcal{E}(k)$, of He⁴. (Hint: There is only one non-degenerate branch of such excitations.)

2. Solar interior: According to astrophysical data, the plasma at the center of the sun has the following properties:

Temperature:	$T = 1.6 \times 10^7 \mathrm{K}$
Hydrogen density:	$\rho_H = 6 \times 10^4 \text{ kg m}^{-3}$
Helium density:	$\rho_{He} = 1 \times 10^5 \text{ kg m}^{-3}.$

(a) Obtain the thermal wavelengths for electrons, protons, and α -particles (nuclei of He).

(b) Assuming that the gas is ideal, determine whether the electron, proton, or α -particle gases are degenerate in the quantum mechanical sense.

(c) Estimate the total gas pressure due to these gas particles near the center of the sun.

(d) Estimate the total radiation pressure close to the center of the sun. Is it matter, or radiation pressure, that prevents the gravitational collapse of the sun?

3. Quantum corrections to the ideal gas: Consider a gas of density n = N/V, composed of identical particles with spin degeneracy g, and kinetic energy $\mathcal{H} = \sum_{i} \frac{\vec{p}_{i}^{2}}{2m}$ in three dimensions. The aim of this problem is to compute the first correction to classical behavior due to quantum (Fermi or Bose) statistics.

(a) Derive the expression for the pressure P(n,T) at temperature T at order of n^2 (i.e. including the second virial coefficient).

(b) Obtain the expression for the energy density E/V to order of n^2 .

(c) Obtain the expression for the heat capacity C_V/N including the first quantum correction, and comment on its behavior for bosons and fermions.

(d) Calculate the expansivity $\alpha_P \equiv \frac{1}{V} \frac{\partial V}{\partial T}\Big|_{P,N}$ to the same order.

(e) Compute the heat capacity C_P/N including the first quantum correction.

4. *Neutron star core:* Professor Rajagopal's group at MIT has proposed that a new phase of QCD matter may exist in the core of neutron stars. This phase can be viewed as a condensate of quarks in which the low energy excitations are approximately

$$\mathcal{E}(\vec{k})_{\pm} =_{\pm} \hbar^2 \frac{\left(|\vec{k}| - k_F\right)^2}{2M}$$

The excitations are fermionic, with a degeneracy of g = 2 from spin.

(a) Assuming a constant density of states near $k = k_F$, i.e. setting $d^3k \approx 4\pi k_F^2 dq$ with $q = |\vec{k}| - k_F$, show that the mean excitation energy of this system at finite temperature is

$$E(T) - E(0) \approx 2gV \frac{k_F^2}{\pi^2} \int_0^\infty dq \frac{\mathcal{E}_+(q)}{\exp\left(\beta \mathcal{E}_+(q)\right) + 1}$$

(b) Give a closed form answer for the excitation energy by evaluating the above integral.

(c) Calculate the heat capacity, C_V , of this system, and comment on its behavior at low temperature.

5. (Optional) Graphene bilayer: The layers of graphite can be peeled apart through different exfoliation processes. Many such processes generate single sheets of carbon atoms, as well as bilayers in which the two sheets are weakly coupled. The hexagonal lattice of the single layer graphene, leads to a band structure that at low energies can be approximated by $\mathcal{E}^{1 \text{ layer}}_{\pm}(\vec{k}) = \pm t_{\parallel}(ak)$, as in relativistic Dirac fermions. (Here $k = |\vec{k}|$, a is a lattice spacing, and t_{\parallel} is a typical in-plane hopping energy.) A weak hopping energy t_{\perp} between the two sheets of the bilayer modifies the low energy excitations drastically, to

$$\mathcal{E}^{\text{bilayer}}_{\pm}(\vec{k}) = \pm \frac{t_{\parallel}^2}{2t_{\perp}} (ka)^2 \quad ,$$

i.e. resembling massive Dirac fermions. In addition to the spin degeneracy, there are two branches of such excitations per unit cell, for an overall degeneracy of g = 4.

(a) For the undoped material with one electron per site, at zero temperature all negative energy states are occupied and all positive energy ones are empty. Find the chemical potential $\mu(T)$.

(b) Show that the mean excitation energy of this system at finite temperature satisfies

$$E(T) - E(0) = 2gA \int \frac{d^2\vec{k}}{(2\pi)^2} \frac{\mathcal{E}_+(\vec{k})}{\exp(\beta \mathcal{E}_+(\vec{k})) + 1}$$

(c) Give a closed form answer for the excitation energy of the bilayer at low temperatures by evaluating the above integral.

(d) Calculate the heat capacity, C_A , of such massive Dirac particles.

(e) A sample contains an equal proportion of single and bilayers. Estimate (in terms of the hopping energies) the temperature below which the electronic heat capacity is dominated by the bilayers.

(f) Explain qualitatively the contribution of phonons (lattice vibrations) to the heat capacity of graphene. The typical sound velocity in graphite is of the order of $2 \times 10^4 \text{ms}^{-1}$.

Is the low temperature heat capacity of (monolayer) graphene controlled by phonon or electron contributions?

6. Density of states: Consider a system of non-interacting identical degrees of freedom, with a set of single-particle energies $\{\varepsilon_n\}$, and ground state $\varepsilon_0 = 0$. In a grand canonical ensemble at temperature $T = (k_B \beta)^{-1}$, the number of particles N is related to the chemical potential μ by

$$N = \sum_{n} \frac{1}{e^{\beta(\varepsilon_n - \mu)} - \eta} = \int_0^\infty d\varepsilon \rho(\varepsilon) \frac{1}{e^{\beta(\varepsilon - \mu)} - \eta}$$

where $\rho(\varepsilon)$ is the density of single-particle states of energy ε , and $\eta = +1(-1)$ for bosons (fermions).

(a) Write a corresponding expression (in terms of $\rho(\varepsilon)$, β , and μ) for the total energy E of the system.

(b) For bosons write an implicit (integral) equation whose solution gives the critical temperature for Bose condensation.

For any function g(x), the Sommerfeld expansion indicates that as $\beta \to \infty$,

$$\int_0^\infty dx \frac{g(x)}{e^{\beta(x-\mu)}+1} \simeq \int_0^\mu dx \ g(x) + \frac{\pi^2}{6\beta^2} \ g'(\mu) + \cdots$$

(c) Use the above expansion to express the low temperature behavior of $\mu - E_F$, where E_F is the Fermi energy, in terms of β , $\rho(E_F)$ and $\rho'(E_F)$.

(d) As in the last part, find an expression for the increase in energy, E(T) - E(T = 0), at low temperatures.

(e) Find the low temperature heat capacity of this system of fermions.

7. Quantum point particle condensation: Consider a quantum gas of N spin-less point particles of mass m at temperature T, and volume V. An unspecified weak pairwise attraction between particles reduces the energy of any state by an amount $-uN^2/(2V)$ with u > 0, such that the partition function is

$$Z(T, N, V) = Z_0(T, N, V) \times \exp\left(\frac{\beta u N^2}{2V}\right),$$

where $Z_0(T, N, V)$ is the partition function of the ideal quantum gas, and $\beta = (k_B T)^{-1}$.

(a) Using the above relation between partition functions relate the pressure P(n,T), as a function of the density n = N/V, to the corresponding pressure $P_0(n,T)$ of an ideal quantum gas.

(b) Use standard results for the non-relativistic gas to show that

$$\frac{\partial P}{\partial n}\Big|_T = -un + k_B T \frac{f_{3/2}^{\eta}(z)}{f_{1/2}^{\eta}(z)}, \quad \text{with} \quad f_{3/2}^{\eta}(z) = n\lambda^3 \quad \text{and} \quad \lambda = \frac{h}{\sqrt{2\pi m k_B T}}.$$

(c) Find the critical value of the coupling $u_c(n,T)$ at which the gas becomes unstable, in the low density (non-degenerate) limit $n\lambda^3 \ll 1$, including the *first* correction that distinguishes between fermi and bose statistics.

(d) For fermions, relate the limiting behavior of $u_c(n, T)$ in the low temperature (degenerate limit $n\lambda^3 \gg 1$) to the fermi energy ϵ_F . (This is somewhat similar to the Chandrashekar instability of neutron stars.)

(e) What happens to u_c for bosons as temperature is decreased towards to quantum degenerate regime?

8. *Harmonic confinement of Fermions:* A classical gas of fermions of mass *m* is confined in a *d*-dimensional anisotropic harmonic potential

$$U(\vec{r}) = \frac{m}{2} \sum_{\alpha} \omega_{\alpha}^2 x_{\alpha}^2 \,,$$

with different restoring frequencies $\{\omega_{\alpha}\}$ along the different directions. We are interested in the limit of wide traps such that $\hbar\omega_{\alpha} \ll k_B T$, and the discreteness of the allowed energies can be ignored.

(a) Show that in this limit, the number of states N(E) with energy less than or equal to E, and the density of states $\rho(E)$, are respectively given by

$$N(E) = \frac{1}{d!} \prod_{\alpha=1}^{d} \left(\frac{E}{\hbar \omega_{\alpha}} \right), \quad \text{and} \quad \rho(E) = \frac{1}{(d-1)!} \frac{E^{d-1}}{\prod_{\alpha} \hbar \omega_{\alpha}}$$

(b) Show that in a grand canonical ensemble, the number of particles in the trap is

$$\langle N \rangle = f_d^-(z) \prod_{\alpha} \left(\frac{k_B T}{\hbar \omega_{\alpha}} \right)$$

(c) Compute the energy of E in the grand canonical ensemble. (Ignore the zero point energy of the oscillators.)

(d) From the limiting forms of the expressions for energy and number, compute the leading term for energy per particle in the high temperature limit.

(e) Compute the limiting value of the chemical potential at zero temperature.

(f) Give the expression for the heat capacity of the gas at low temperatures, correct up to numerical factors that you need not compute.

9. (Optional) Bose condensation with trap sites: With the aid of an 'optical lattice', a density ρ of trapping sites is created within a volume containing a density n of identical and non-interacting bosons. Each trap site can either be empty, or contain one (and only one) Bose particle. Assume that a trapped particle is completely localized to the site and can be treated as a classical particle of energy $\epsilon = -w < 0$ (i.e., energy is lowered by w upon trapping). We further assume that the trapping sites have no effect on the spectrum of the non-trapped particles, which can be treated as an ideal gas with single particle states of kinetic energy $(\hbar \vec{k})^2/2m$.

(a) In a grand canonical ensemble of chemical potential μ and temperature T, what is the density n_t of trapped particles.

(b) What is the density n_g of gas particles as a function of μ , T, the mass m and spin degeneracy g of the bosons?

(c) Obtain the critical (total) density $n^*(T)$ for the onset of Bose–Einsten condensation, and sketch it for a small value of w.

(d) Write the expression for the total energy density in the Bose condensed phase.

10. (Optional) Ring diagrams mimicking bosons: Motivated by the statistical attraction between bosons, consider a classical system of identical particles, interacting with a pairwise potential $V(|\vec{q} - \vec{q}'|)$, such that

$$f(\vec{r}) = e^{-\beta V(r)} - 1 = \exp\left(-\frac{\pi r^2}{\lambda^2}\right)$$
, and $\tilde{f}(\vec{\omega}) = \lambda^3 \exp\left(-\frac{\lambda^2 \omega^2}{4\pi}\right)$,

where $\tilde{f}(\vec{\omega})$ is the Fourier transform of $f(\vec{r})$.

(a) In a perturbative cluster expansion of the partition function, we shall retain only the diagrams forming a ring, which (after a summation over all powers of V between any pair of points) are proportional to

$$R_{\ell} = \int \frac{d^3 \vec{q_1}}{V} \cdots \frac{d^3 \vec{q_{\ell}}}{V} f(\vec{q_1} - \vec{q_2}) f(\vec{q_2} - \vec{q_3}) \cdots f(\vec{q_{\ell}} - \vec{q_1}).$$

Use properties of Fourier transforms to show that

$$R_{\ell} = \frac{1}{V^{\ell-1}} \int \frac{d^3 \vec{\omega}}{(2\pi)^3} \, \tilde{f}(\vec{\omega})^{\ell} = \frac{\lambda^{3\ell}}{\ell^{3/2} \lambda^3 V^{\ell-1}} \, .$$

(b) Show that in the ring approximation, the partition function is given by

$$\ln Z_{\rm rings} = \ln Z_0 + \frac{V}{2\lambda^3} f_{5/2}^+(n\lambda^3) - \frac{N}{2} + \frac{N^2\lambda^3}{2V} (1 - 2^{-5/2}),$$

where Z_0 is the partition function of the non-interacting gas, and n = N/V is the number density.

(c) Compute the pressure P of the gas within the ring approximation.

(d) By examining the compressibility, or equivalently $\partial P/\partial n|_T$, show that this classical system of interacting particles must undergo a condensation transition.

11. (Optional) Bose condensation in d-dimensions: Consider a gas of non-interacting (spinless) bosons with an energy spectrum $\epsilon = p^2/2m$, contained in a box of "volume" $V = L^d$ in d dimensions.

(a) Calculate the grand potential $\mathcal{G} = -k_B T \ln \mathcal{Q}$, and the density n = N/V, at a chemical potential μ . Express your answers in terms of d and $f_m^+(z)$, where $z = e^{\beta\mu}$, and

$$f_{m}^{+}(z) = \frac{1}{\Gamma(m)} \int_{0}^{\infty} \frac{x^{m-1}}{z^{-1}e^{x} - 1} dx.$$

(Hint: Use integration by parts on the expression for $\ln Q$.)

(b) Calculate the ratio PV/E, and compare it to the classical value.

(c) Find the critical temperature, $T_c(n)$, for Bose-Einstein condensation.

(d) Calculate the heat capacity C(T) for $T < T_c(n)$.

(e) Sketch the heat capacity at all temperatures.

(f) Find the ratio, $C_{\text{max}}/C(T \to \infty)$, of the maximum heat capacity to its classical limit, and evaluate it in d = 3.

(g) How does the above calculated ratio behave as $d \rightarrow 2$? In what dimensions are your results valid? Explain.

12. (**Optional**) *Surface adsorption of an ideal Bose gas:* Consider adsorption of particles of an ideal (spin-less) Bose gas onto a two dimensional surface.

(a) Treating the ambient gas as a *non-degenerate* ideal gas of temperature T and pressure P, find its chemical potential $\mu(T, P)$.

(b) The gas is in contact with a attractive surface, such that a particle gains an energy u upon adsorption to the surface. Treating the particles on the surface as a two dimensional ideal gas (in equilibrium with the ambient gas), find the areal density n_2 as a function of P, u, and temperature $(T, \beta, \text{ and/or } \lambda)$.

(c) Find the maximum pressure P^* before complete condensation to the surface.

(d) Find the singular behavior of n_2 for $\delta P = P^* - P \rightarrow 0$.

13. (Optional) Inertia of superfluid helium: Changes in frequency of a torsional oscillator immersed in liquid helium can be used to track the "normal fraction" of the liquid as a function of temperature. This problem aims at computing the contribution of phonons (dominant at low temperatures) to the fraction of superfluid that moves with the oscillator plates. Consider a superfluid confined between two parallel plates moving with velocity \vec{v} . (a) The isolated stationary superfluid has a branch of low energy excitations characterized by energy $\epsilon(p)$, where $p = |\vec{p}|$ is the magnitude of the momentum \vec{p} . Show that for excitations produced by walls (of large mass M) moving with velocity \vec{v} , this spectrum is modified (due to consideration of momentum and energy of the walls) to $\epsilon_{\vec{v}}(\vec{p}) = \epsilon(p) - \vec{p} \cdot \vec{v}$. (b) Using the standard Bose occupation number for particles of energy $\epsilon_{\vec{v}}(\vec{p})$, obtain an integral expression for the net momentum \vec{P} carried by the excitations in the superfluid. (**Hint:** $\sum_{\vec{p}} = V \int d^3 \vec{p} / h^3$, where V is the volume.)

(c) Expanding the result for small velocities, show that $P_{\alpha} = V \rho_n v_{\alpha}$, and give an integral expression for ρ_n . (Hint: The angular average of $p_{\alpha} p_{\gamma}$ is $p^2 \delta_{\alpha\gamma}/3$.)

(d) Compute the contribution of phonons, with $\epsilon(p) = cp$, to ρ_n . (An answer that is correct up to a numerical coefficient is sufficient.)

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