1. For rotations of a single diatomic molecule, the quantum partition function is

\[
z_{\text{rot}} = \sum_{j=0}^{\infty} \sum_{m_j=-j}^{j} e^{-\varepsilon_j/kT}, \quad \varepsilon_j = \frac{J^2}{2I}, \quad J^2 = j(j+1)\hbar^2
\]

where \(m_j = -j, -j+1, \ldots, 0, \ldots, j-1, j\) has \((2j+1)\) values.

(a) (7) For \(kT \gg \hbar^2/2I\), the summand is a slowly varying function, so you can approximately replace the sum by an integral. Do this (correctly), and then evaluate the integral to obtain \(z_{\text{rot}}\) as a function of temperature.

(b) (6) Use your answer to part (a) to obtain the rotational energy \(\varepsilon_{\text{rot}}\) per molecule as a function of temperature.

(c) (6) Now consider a **classical** model of diatomic molecules. You may assume that a canonical transformation has been performed from the original atomic coordinates to the relative coordinate \(\vec{r} = \vec{r}_1 - \vec{r}_2\) and the center of mass coordinate \(\vec{R}\). Also assume that \(\vec{r}\) has been transformed to spherical coordinates \(r, \theta, \phi\) (which is again a canonical transformation). Finally, assume that the vibrations are small enough that (i) the rotational moments of inertia can be taken to be constant, (ii) the above harmonic approximation is valid, and (iii) you may take the limits of integration for the displacement

\[u = r - r_0\]

to be \(\pm \infty\). (Here \(r_0\) is the equilibrium value of the "bond length" \(r\). We are also assuming a high enough temperature for classical mechanics to be valid.)

The original Hamiltonian for atoms 1 and 2 is

\[H = \frac{1}{2m}(p_1^2 + p_2^2) + \frac{1}{2}Ku^2\]

where again \(u = r - r_0\) is the displacement from equilibrium. In this part of the problem, use the **procedure for calculating the average value of an arbitrary quantity in classical statistical mechanics** to obtain \(\langle u^2 \rangle\), the average value of \(u^2\), as a function of the temperature \(T\).
Recall that the classical average value of a quantity $A$ (for one molecule) is given by

$$\langle A \rangle = \frac{1}{z} \int dp \, dq \, A \, e^{-H(p,q)/kT}, \quad z = \int dp \, dq \, e^{-H(p,q)/kT}$$

where $p$ and $q$ represent all the momenta and coordinates, so that $\int dp \, dq$ represents an integral over all of the momentum components and all of the coordinates. But you can quickly argue that most of the integrals will cancel in the numerator and denominator when you are calculating $\langle u^2 \rangle$.

(d) (6) Now obtain $\langle u^2 \rangle$ from the equipartition theorem. Do the results agree?
2. The simplest Ginzburg-Landau free energy has the form

\[ F = a(T - T_c)\psi^2 + \frac{1}{2}b\psi^4 \]

where \( \psi \) is a real order parameter. (The true power of Ginzburg-Landau is its ability to treat complex order parameters – “macroscopic wavefunctions”– and couplings to the electromagnetic and other gauge fields, but those topics are beyond the present treatment.)

(a) (6) Show that there is a phase transition as \( T \) is lowered, to a state with a nonzero order parameter below \( T_c \).

Obtain the equilibrium free energy for \( T < T_c \) as well as \( T > T_c \).

(b) (6) Show that there is a jump in the heat capacity \( C_V \) at \( T = T_c \), and calculate its value in terms of the constants above.

(c) (6) For the BCS theory of superconductivity, we showed (in a slightly different notation) that

\[ C_V = -2k \beta_c \rho(\varepsilon_F) \left[ \varepsilon_F^2 + \frac{1}{2}\beta_c \left( \frac{\partial\Delta^2}{\partial\beta} \right)_{T_c} \right] , \quad \beta = \frac{1}{kT} , \quad \beta_c = \frac{1}{kT_c} \]

where \( \Delta \) is the gap function, with \( E^2 = \varepsilon^2 + \Delta^2 \) for a Bogoliubov quasiparticle.

Show that there is a jump in the heat capacity \( C_V \) at \( T = T_c \), and obtain its value in terms of the constants above and \( (\partial\Delta^2/\partial T)_{T_c} \).

Also, sketch a graph of the BCS \( \Delta(T) \) as a function of the temperature \( T \).

(d) (6) Ginzburg-Landau mean-field theory is a good approximation for superconductors, superfluid \( ^3\text{He} \), and some magnetic systems, plus charge density waves, spin density waves, etc., but it fails for other (experimental and theoretical) systems including superfluid \( ^4\text{He} \) and the 2-dimensional Ising model. For this theoretical model we obtained the approximate result that the critical exponent \( \alpha \) in

\[ C_V \propto |T - T_c|^{-\alpha} \quad \text{for } T \approx T_c \]

is given by

\[ 2 = \left[ \frac{dK'}{dK} \right]^{2-\alpha}_{K=K_c} \quad \text{with} \quad K_c = 0.507 \quad \text{and} \quad K' = \frac{3}{8} \ln \cosh(4K) . \]
Obtain the expression for $\alpha$ in terms of a standard hyperbolic function at $K = K_c$.

(e) (1) Obtain the numerical value of the critical exponent $\alpha$ by evaluating your expression in part (d). A calculator will be provided. (Enter the argument and then press HYP before SIN, COS, or TAN to get the value of the sinh, cosh, or tanh of that argument.)
3. In this problem we calculate the sound velocities $u_F$ in a Fermi gas and $u_B$ in a Bose gas at $T = 0$, using

$$u = \left( \frac{\partial P}{\partial \rho_m} \right)^{1/2}_S = \left( \frac{1}{mn \kappa_s} \right)^{1/2}_S$$

where $\rho_m$ is the mass density, $n = N/V$ is the number density, and $m$ is the mass of a particle. You may use the fact that for a (3-dimensional nonrelativistic) quantum ideal gas, the (single-particle) density of states has the form

$$\rho(\varepsilon) = AV\varepsilon^{1/2}$$

where $A$ is a constant and $V$ is the volume.

(The calculations below are to be done for ideal quantum gases, with the understanding that true sound waves actually require some interaction between particles.)

**First the Fermi gas:** Using Euler’s theorem and the original expression for $dE$, we obtained the Gibbs-Duhem relation, which you can just assume in working this problem:

$$-SdT + VdP - Nd\mu = 0 .$$

(a) (5) Rewrite the Gibbs-Duhem relation in terms of $s \equiv S/N$ and $n \equiv N/V$. Then obtain the relation between $(\partial \mu/\partial n)_T$ and $(\partial P/\partial n)_T$.

(b) (5) Although the sound velocity $u_F$ is given by the equation above,

$$u_F^2 = \left( \frac{1}{mn \kappa_s} \right),$$

we will calculate it at $T = 0$, where $S = 0$:

$$u_F^2 = \left( \frac{1}{mn \kappa_T} \right) = \frac{1}{m} \left( \frac{\partial P}{\partial n} \right)_T \text{ for } T = 0 .$$

Starting with this equation, and using the result of part (a), obtain $u_F$ (at $T = 0$) in terms of $(\partial \varepsilon_F/\partial n)_T$, where $\varepsilon_F = \mu (T = 0)$ is the Fermi energy.

(c) (5) Using the density of states function $\rho(\varepsilon)$ above, calculate $\varepsilon_F$ in terms of $n = N/V$ and the constant $A$. 


(d) (5) Using your results of parts (b) and (c), calculate \( u_F \) and obtain its relation to the Fermi velocity \( v_F \), defined by \( \varepsilon_F = \frac{1}{2}mv_F^2 \).

(e) (5) Let us check the consistency of our assumption in part (b) that \( \kappa_S = \kappa_T \) at \( T = 0 \), using the thermodynamic relation

\[
\frac{\kappa_T}{\kappa_S} = \gamma \equiv \frac{C_P}{C_V}
\]

with

\[
\gamma = \frac{5}{3} \frac{f_{5/2}(\lambda) f_{1/2}(\lambda)}{[f_{3/2}(\lambda)]^2}, \quad \lambda \equiv e^{\mu/kT}
\]

\[
f_\nu(e^\xi) = \frac{\xi^\nu}{\Gamma(\nu + 1)} \left[ 1 + \nu(\nu - 1) \frac{\pi^2}{6} \frac{1}{\xi^2} + \ldots \right], \quad \Gamma(1/2) = \pi^{1/2}.
\]

Calculate \( \gamma \) to first order in \( (kT/\varepsilon_F)^2 \) and check whether \( \kappa_S = \kappa_T \) at \( T = 0 \).

(f) (5) **Now the Bose gas:** For \( T < T_c \) (the critical temperature), \( \lambda \equiv e^{\mu/kT} \) has a specific fixed value. Use this fact, and the result of part (a), and the fact that

\[
u_B = \left( \frac{1}{mn\kappa_T} \right)^{1/2} = \frac{1}{m^{1/2}} \left( \frac{\partial P}{\partial n} \right)^{1/2}_T \quad \text{for } T = 0
\]

to calculate this “sound velocity” of an ideal Bose gas at \( T = 0 \).
4. Let us consider the general problem of an ideal relativistic ideal gas of bosons in $D$ dimensions, so that the energy $\varepsilon$ is related to the magnitude $p$ of the momentum by

$$\varepsilon(p) = cp.$$ 

(a) (15) Determine the largest value of $D$ for which there is no Bose-Einstein condensation for $T > 0$.

[Hint: Determine the density of states in momentum space, $\rho(p)$, and then as a function of energy, $\rho(\varepsilon)$. Next write $N - N_0$ as an integral involving the density of states function and the Bose-Einstein distribution function with $\mu \to 0$. Here $N_0$ is the number of particles in the condensate that is required by mathematical consistency. Finally, demonstrate (convincingly) that the integral diverges for some values of $D$ and converges for other values. To demonstrate convergence or divergence, focus on the behavior of the integrand at the lower limit of integration.]

(b) (5) How does this result compare with the one which we learned for nonrelativistic bosons?