Reduce sums over orbitals to integrals over orbital energy ε

a)
$$\varepsilon = (p_x^2 + p_y^2 + p_z^2)/2m$$
:

$$\int dp_x dp_y dp_z = 2\pi (2m)^{3/2} \int_0^\infty d\varepsilon \ \varepsilon^{1/2}$$

b)
$$\varepsilon = \sqrt{p_x^2 + p_y^2 + p_z^2} \ c$$
:

$$\int dp_x dp_y dp_z = \frac{4\pi}{c^3} \int_0^\infty d\varepsilon \ \varepsilon^2$$

c)
$$\varepsilon = (p_x^2 + p_y^2 + p_z^2)/2m + m\omega^2(x^2 + y^2 + z^2)/2$$
:

$$\int dx dy dz \int dp_x dp_y dp_z = \frac{1}{2} \left(\frac{2\pi}{\omega}\right)^3 \int_0^\infty d\varepsilon \ \varepsilon^2$$

Integral tables

$$\int_0^\infty dt \frac{t^n}{e^t - 1} = \frac{\sqrt{\pi}\zeta(3/2)}{2}, \ \frac{\pi^2}{6}, \ \frac{3\sqrt{\pi}\zeta(5/2)}{4}, \ 2\zeta(3), \ \frac{\pi^4}{15}$$
for $n = \frac{1}{2}, 1, \frac{3}{2}, 2, 3$

$$\int_{0}^{\infty} dt \frac{t^{n}}{e^{t}+1} = 1, \frac{(2-\sqrt{2})\sqrt{\pi}\zeta(3/2)}{4}, \frac{\pi^{2}}{12}, frac3(4-\sqrt{2})\sqrt{\pi}\zeta(5/2)16, \frac{3\zeta(3)}{2}, \frac{7\pi^{4}}{120}$$
 for $n = \frac{1}{2}, 1, \frac{3}{2}, 2, 3$

$$\int_0^\infty dt \ t^n e^{-t} = \frac{\sqrt{\pi}}{2}, \ 1, \ \frac{3\sqrt{\pi}}{4}, \ 2, \ 6$$
for $n = \frac{1}{2}, \ 1, \ \frac{3}{2}, \ 2, \ 3$

Problem 1.

Three of the most important ensembles in statistical physics are

M. microcanonical ensemble with N particles and total energy U

C. canonical ensemble with N particles at temperature T

G. grand canonical ensemble at chemical potential μ and temperature T

In the microcanonical ensemble, the normalized probability distribution for the microstates is

$$P_s = 1/\Omega(U)$$
 if $U_s = U$
= 0 if $U_s \neq U$
 $\Omega(U) =$ multiplicity of microstates with total energy U

(A) What is the normalized probability distribution for the canonical ensemble (C)? (Define any variables you introduce.)

(B) What is the normalized probability distribution for the grand canonical ensemble (G)?

$$P_s = \frac{1}{Z} e^{-\beta(U_s - \mu N_s)}$$
 $Z = \overline{Z} e^{-\beta(U_s - \mu N_s)}$

The following three systems each consists of a gas with N molecules (at least on average) and with total energy U (at least on average) in a box of volume V with different environments.

system 1: the box is surrounded by thermal insulation. system 2: the box has thermally conducting walls and is

inside a much larger box containing a gas of the same molecules.

system 3: the box is just a region of volume V with no walls

inside a much larger box containing a gas of the same molecules.

(C) For each of the three systems 1, 2, and 3, list which (if any) of the quantities U and N is conserved:

system 1: U, N system 2: U system 3: neither

(D) For each of the three systems, list the ensembles (M, C, G) that according to the Fundamental Assumption of Statistical Physics describe the equilibrium macroscopic behavior of the system (including fluctuations in N and U).

system 1: M

system 2: C

system 3: G

(E) For each of the three systems, list the ensembles (M, C, G) that describe the equilibrium macroscopic behavior of the system in the thermodynamic limit $V \to \infty$ with N/V, U/V fixed.

system 1: M, C, G

system 2: M, C, G

system 3: M, C, G

Problem 2.

A large number N of <u>bosonic</u> atoms, all in the same spin state, are trapped in a 3-dimensional harmonic oscillator potential: $V(r) = \frac{1}{2}m\omega^2r^2$. The lowest orbital has energy $\varepsilon_0 = \frac{3}{2}\hbar\omega$. Let T_c be the critical temperature for Bose-Einstein condensation of the atoms.

(A) For $T > T_c$, write down general expressions for N and the total energy U of the atoms in the form of definite integrals over the orbital energy ε .

$$N = \frac{1}{h^3} \int d^3r \int d^3p \frac{1}{e^{\beta(\epsilon-\mu)} - 1} = \frac{1}{h^3} \frac{1}{2} \left(\frac{2\pi}{\omega}\right)^3 \int_0^{\infty} d\epsilon \frac{\epsilon^2}{e^{\beta(\epsilon-\mu)} - 1}$$

$$U = \frac{1}{h^3} \int d^3r \int d^3p \frac{\epsilon}{e^{\beta(\epsilon-\mu)} - 1} = \frac{1}{h^3} \frac{1}{2} \left(\frac{2\pi}{\omega}\right)^3 \int_0^{\infty} d\epsilon \frac{\epsilon^3}{e^{\beta(\epsilon-\mu)} - 1}$$

(B) For $T < T_c$, write down expressions for N and U in terms of the number of atoms in the Bose-Einstein condensate N_0 (instead of the chemical potential) and an integral that depends on T.

$$N = N_0 + \frac{1}{h^3} \int_0^3 r \int_0^3 p \frac{1}{e^{\beta \epsilon} - 1} = N_0 + \frac{1}{h^3} \frac{1}{2} \left(\frac{2\pi}{\omega}\right)^3 \int_0^3 d\epsilon \frac{\epsilon^2}{e^{\beta \epsilon} - 1}$$

$$U = N_0 \epsilon_0 + \frac{1}{h^3} \int_0^3 r \int_0^3 p \frac{1}{e^{\beta \epsilon} - 1} = N_0 \left(\frac{2}{2} t \omega\right) + \frac{1}{h^3} \frac{1}{2} \left(\frac{2\pi}{\omega}\right)^3 \int_0^3 d\epsilon \frac{\epsilon^3}{e^{\beta \epsilon} - 1}$$

(C) Deduce the critical temperature T_c as a function of N and ω .

$$N = \frac{1}{2h^3} \left(\frac{2\pi}{\omega}\right)^3 \int_0^{\infty} d\epsilon \frac{\epsilon^2}{e^{\beta\epsilon} - 1} = \frac{1}{2} \left(\frac{2\pi}{h\omega}\right)^3 \frac{1}{\beta^3} \int_0^{\infty} dt \frac{t^2}{e^{t} - 1} t = \beta\epsilon$$

$$= \frac{1}{2} \left(\frac{2\pi}{h\omega}\right)^3 (kT)^3 \cdot 25(3) = 5(3) \left(\frac{2\pi}{h\omega}\right)^3 (kT)^3$$

$$kT_c = \left(\frac{N}{S/3}\right)^{\frac{1}{3}} \frac{h\omega}{2\pi}$$

(D) For $T < T_c$, deduce the condensate fraction N_0/N as a function of T, N, and ω (or T/T_c).

$$N = N_0 + \frac{1}{2} \left(\frac{2\pi}{h\omega}\right)^3 \int_0^\infty d\epsilon \frac{\epsilon^2}{e^{\beta\epsilon} - 1}$$

$$= N_0 + \frac{1}{2} \left(\frac{2\pi}{h\omega}\right)^3 2 3(3) (kT)^3$$

$$= N_0 + N \left(\frac{T}{T_c}\right)^3$$

$$N_0 = N \left[1 - \left(\frac{T}{T_c}\right)^3\right]$$

$$\frac{N_0}{N} = 1 - \left(\frac{T}{T_c}\right)^3$$

Problem 3.

In the interior of a white dwarf star, the electrons are effectively at zero temperature. They can be relativistic with energies $\varepsilon = \sqrt{m_e^2 c^4 + p^2 c^2}$. Electrons have two spin states.

(A) Draw a graph of the occupation number $n(\varepsilon)$ of the electrons as a function of the orbital energy ε . Indicate the rest mass $m_e c^2$ and the Fermi energy ϵ_F on the graph.



Suppose the electrons are ultrarelativistic with energies $\varepsilon = pc$.

(B) Write down an expression for the number N of electrons in a volume V in the form of a simple integral over the orbital energy ε .

$$N = 2 \frac{1}{h^3} \int d^3r \int d^3p = \frac{2}{h^3} V \frac{4\pi}{c^3} \int_0^{\epsilon_p} d\epsilon \, \epsilon^2 = \frac{8\pi V}{h^3 c^3} \int_0^{\epsilon_p} d\epsilon \, \epsilon^2$$

(C) Determine the Fermi energy ϵ_F as a function of N and V (and the fundamental constants h and m_e).

$$N = \frac{8\pi V}{h^3 c^3} \frac{\epsilon_F^3}{3}$$

$$\epsilon_F = \left(\frac{3h^3c^3N}{8\pi V}\right)^{V_3} = \left(\frac{3}{8\pi}\frac{N}{V}\right)^{1/3}$$

Suppose the electrons are nonrelativistic with energies $\varepsilon = m_e c^2 + p^2/2m_e$.

(E) Write down an expression for N in terms of a simple integral over the orbital energy ε (or perhaps the kinetic energy $\varepsilon_{\rm kin} = \varepsilon - m_e c^2$).

erhaps the kinetic energy
$$\varepsilon_{kin} = \varepsilon - m_e c^2$$
.

$$N = 2 \frac{1}{h^3} \int d^3 r \int d^3 p = \frac{2}{h^3} V 2\pi (2m)^{3/2} \int_{m_e c^2}^{\epsilon_F} d\epsilon (\epsilon - m_e c^2)^{V_2} = \frac{4\pi V (2m)^{3/2}}{h^3} \int d\epsilon' (\epsilon')^{V_2}$$

E) Determine the Fermi energy ϵ_F as a function of N and V

(F) Determine the Fermi energy ϵ_F as a function of N and V.

$$N = \frac{4\pi \sqrt{(2m)^{3/2}}}{h^3} \frac{(\epsilon_F - m_e c^2)^{3/2}}{\frac{3/2}}$$

$$= \frac{8\pi \sqrt{(2m)^{3/2}}(\epsilon_F - m_e c^2)^{3/2}}{\frac{3}{4}}$$

$$\epsilon_{\rm F} - m_{\rm e}c^2 = \left(\frac{3h^3N}{8\pi V(2m)^{3/2}}\right)^{2/3}$$

$$E_P = m_e c^2 + \left(\frac{3}{8\pi} \frac{N}{V}\right)^{2/3} \frac{h^2}{2m}$$

Problem 4.

The spectrum of black-body radiation can be derived by considering either standing electromagnetic waves or a gas of photons inside a cavity in a conductor.

The normal modes of standing EM waves in a cube of volume L^3 can be labelled by integers $n_x, n_y, n_z = 1, 2, 3, \ldots$ The amplitude a of a normal mode oscillates with frequency $f = \sqrt{n_x^2 + n_y^2 + n_z^2} c/2L$. Its energy E is determined by a and its time derivative \dot{a} : $E \propto \dot{a}^2 + 4\pi^2 f^2 a^2$. If a sum over the normal modes is dominated by high frequencies, it can be approximated by an integral over the frequency:

$$2\sum_{n_x=1}^{\infty} \sum_{n_y=1}^{\infty} \sum_{n_z=1}^{\infty} \approx (8\pi L^3/c^3) \int_0^{\infty} df \ f^2.$$

(A) Suppose the standing EM waves are in equilibrium at temperature T and can be treated using the canonical ensemble. Use the equipartition theorem to determine the average energy \bar{E} in a single normal mode.

2 quadratu degrees of freedom: a, a equipartition theorem $\overline{B} = 2.1 + T = kT$

(B) Express the total energy U of the standing EM waves as an integral over the frequency f. Explain what is meant by the phrase "ultraviolet catastrophe".

$$U = 2\sum_{n=1}^{\infty} \sum_{n=1}^{\infty} \sum_{n=1}^{\infty} kT = \frac{8\pi L^3}{c^3} kT \int_0^{\infty} df f^2$$

The catastrophe is that the integral over f is infinite.

It is an intraviolet constastrople because the divergence come from the large of region, which is ultraviolet (C) Planck explained the spectrum of black body radiation by assuming that the energy in each normal mode is quantized, with the energy quantum proportional to the frequency: E = nhf, $n = 0, 1, 2, \ldots$ Given this additional assumption, express the average energy E in the normal mode as a ratio of sums over n.

The Bultymann factor for E=nhf is e-Buhf The average energy is $\overline{B} = \frac{\sum_{n=0}^{\infty} nhf e^{-\beta nhf}}{\sum_{n=0}^{\infty} e^{-\beta nhf}} \qquad \left(\overline{B} = \frac{hf}{e^{\beta hf} - 1}\right)$

(D) Express the total energy U of the standing EM waves as an integral over the frequency f.

$$U = 2\sum_{n_1=1}^{\infty}\sum_{n_2=1}^{\infty}\overline{E} = \frac{8\pi L^3}{c^3}\int_0^{\infty}df\,f^2\,\overline{E}$$

$$\left(U = \frac{8\pi L^3}{c^3} \int_0^\infty df \, f^2 \frac{hf}{e^{\beta hf} - 1}\right)$$

(E) Bose explained the spectrum of black body radiation by assuming that the cavity contains an ideal gas of identical bosons (photons) with energy E = hf, momentum p = hf/c, and chemical potential $\mu = 0$. Identify a reaction that would guarantee $\mu = 0$ by chemical equilibrium. atom () atom + photor

$$U = 2\frac{1}{h^3}\int_{0}^{3}r\int_{0}^{3}p\frac{\epsilon}{e^{\beta\epsilon}-1} = \frac{2}{h^3}V\frac{4\pi}{c^3}\int_{0}^{\infty}d\epsilon \epsilon^2\frac{\epsilon}{e^{\beta\epsilon}-1}$$

$$= \frac{8\pi V}{h^3c^3}h^4\int_{0}^{\infty}df\frac{f^3}{e^{\beta hf}-1} = \frac{8\pi Vh}{c^3}\int_{0}^{\infty}df\frac{f^3}{e^{\beta hf}-1}$$