Statistical Physics (PHY831), Part 2-Exact results and solvable models

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Systems that will be covered include:(11 lectures)
Classical ideal gas, Non-interacting spin systems, Harmonic oscillators, Energy levels of a non-relativistic and relavistic particle in a box, ideal Bose and Fermi gases. One dimensional and infinite range ising models. Applications to atom traps, white dwarf and neutron stars, electrons in metals, photons and solar energy, phonons, Bose condensation and superfluidity, the early universe.

Midterm 2, Lecture 22 (Friday Oct. 21)

I.   CLASSICAL AND QUANTUM IDEAL GASES - SOLVABLE CASES

A.   Classical systems with a Maxwell-Boltzmann distribution of velocities

The Hamiltonian for a classical particle system with interactions that only depend on the particle co-ordinates is,

$$H = \sum_{i=1}^{N} \frac{\vec{p}_i^2}{2m} + V_r(\{\vec{r}_i\}). \tag{1}$$

In classical particle systems the Hamiltonian or Energy can often be approximated by pair interactions, so that

$$H = KE + V_r = \sum_{i=1}^{N} \frac{\vec{p}_i^2}{2m} + \sum_{i>j}^{N} V_2(\vec{r}_{ij}). \tag{2}$$

In the cannonical ensemble for systems with Hamiltonian (1), the probability of finding a particle at a point in phase space is given by,

$$p = Ae^{-\beta H} = Ae^{-\beta(KE+V_r)} = A_{KE}e^{-\beta KE}A_r e^{-\beta V_r} = p_r p_v. \tag{3}$$

That is, the Boltzmann probabilitiy factors into a part that contains the potential and a part that contains the momentum. The momentum part of the Hamilonian is simply $\sum_i \vec{p}_i^2/2m$. Now note that p_v also factors, i.e. $p_v = p_{v_1}...p_{v_N}$ and the probability of finding any one particle in a momentum state $\vec{p}_i$ is then,

$$p_{MB}(\vec{p}_i) = A_1 e^{-\beta \frac{\vec{p}_i^2}{2m}} = \left(\frac{\beta}{2m\pi}\right)^{3/2} e^{-\frac{\vec{p}_i^2}{2mk_BT}}. \tag{4}$$

This expression holds for every particle in the system. Often this is written in terms of the velocities

$$p_{MB}(\vec{v}) = \left(\frac{m\beta}{2\pi}\right)^{3/2} e^{-\frac{m\vec{v}^2}{2k_BT}} \tag{5}$$

where the prefactor is found by normalizing the probability. From this "Maxwell-Boltzmann" distribution it is easy to show that the root mean square velocity of particles is related to the temperature through

$$\frac{1}{2}m < \vec{v}^2 > = \frac{3}{2}k_BT \quad \text{or} \quad < KE > = \frac{3}{2}Nk_BT \quad \text{for a monatomic system} \tag{6}$$

This is the equipartition theorem for a monatomic system. More generally, the kinetic energy per degree of freedom is $\frac{1}{2}k_BT$. For an ideal gas the kinetic energy and the internal energy are the same. However for an interacting system the internal energy is the kinetic plus potential energy, so the equipartition result applies to the kinetic energy for systems with interactions that are momentum independent.

B.   Classical ideal gas in a box with volume $V = L^3$, phase space method

Since there are no interactions in the ideal gas, the equipartition theorem gives the internal energy of an ideal monatomic gas in three dimensions $U = 3Nk_BT/2$. This is not sufficient for us to find all of the thermodynamics as for that we need $U(S, V, N)$. To find all of the thermodynamics, we can work in the microcanonical, canonical or grand canonical ensembles. First lets look at the canonical ensemble.

To find the canonical partition function, we consider the phase space integral for N monatomic particles in a volume V at temperature T, so that,

$$Z = \frac{1}{N!h^{3N}} \int dq_1^3...dq_N^3 \int dp_1^3....dp_n^3 e^{-\beta H}. \tag{7}$$

where H is the Hamiltonian, that for a non-interacting gas is simply $H = \sum_i \vec{p}_i^2/2m$. The prefactor $1/(N!h^{3N})$ are due to the Gibb's paradox and Heisenberg uncertainty principle respectively. The Gibb's paradox notes that if we integrate over all positions for each particle, we overcount the configurations of identical particles. That is we count the $N!$ ways of arranging the particles. This factor should only be counted if the particles are distinguishable. The factor $1/h^{3N}$ is due to the uncertainty relation $\delta x \delta p > \hbar/2$, which states that the smallest region of phase space that makes sense quantum mechanically is $\hbar^3/8$. The fact that the normalization is $1/h^3$ per particle is to ensure that the classical or Maxwell-Boltzmann gas defined above agrees with the high temperature behavior of the ideal Bose and Fermi gases, as we shall show later.

For an ideal gas, the integrals over position in (7) give V^N, while the integrals over momenta separate into $3N$ Gaussian integrals, so that,

$$Z = \frac{V^N}{N!h^{3N}} I^{3N} \quad \text{where} \quad I = \int_{-\infty}^{\infty} e^{-\beta p^2/2m} = \left(\frac{2m\pi}{\beta}\right)^{1/2}. \tag{8}$$

This may be written as,

$$Z = \frac{V^N}{\lambda^{3N} N!} \quad \text{where} \quad \lambda = \left(\frac{h^2}{2\pi m k_B T}\right)^{1/2} \tag{9}$$

is the thermal de Broglie wavelength. Note that the partition function is dimensionless. The thermal de Broglie wavelength is an important length scale in gases. If the average interparticle spacing, $L_c = (V/N)^{1/3}$ is less than λ quantum effects are important, while if $L_c > \lambda$, the gas can be treated as a classical gas. We shall use this parameter later to decide if particles in atom traps are expected to behave as classical or quantum systems. The thermal de Broglie wavelength of Eq. (9) is for massive particles with a free particle dispersion relation, that is $\epsilon(p) \propto \vec{p}^2$. For massless particles or particles with different dispersion relations, a modified de Broglie wavelength needs to be defined. From the canonical partition function we find the Helmholtz free energy,

$$F = -k_B T ln(Z) = -k_B T ln(\frac{V^N}{\lambda^{3N} N!}) \tag{10}$$

This expression is in terms of its natural variables $F(T, V, N)$, so we can find all of the thermodynamics from it as follows:

$$dF = -SdT - PdV + \mu dN = \left(\frac{\partial F}{\partial T}\right)_{V,N} dT + \left(\frac{\partial F}{\partial V}\right)_{T,N} dV + \left(\frac{\partial F}{\partial N}\right)_{T,V} dN \tag{11}$$

and hence

$$S = -\left(\frac{\partial F}{\partial T}\right)_{V,N} = k_B ln(\frac{V^N}{\lambda^{3N} N!}) + \frac{3}{2} N k_B \tag{12}$$

The internal energy is found by combining (10) and (12), so that,

$$U = F + TS = \frac{3}{2} N k_B T \tag{13}$$

The pressure is given by,

$$P = -\left(\frac{\partial F}{\partial V}\right)_{T,N} = k_B T \frac{N}{V} = \frac{k_B N T}{V}, \tag{14}$$

which is the ideal gas law, while the chemical potential is,

$$\mu = \left(\frac{\partial F}{\partial N}\right)_{T,V} = k_B T ln(\lambda^3 N/V) \tag{15}$$

The response functions are then,

$$C_V \left(\frac{\partial U}{\partial T}\right)_{V,N} = \frac{3Nk_B}{2}, \quad C_P = \left(\frac{\partial H}{\partial T}\right)_{P,N} = \frac{5Nk_B}{2} \tag{16}$$

where we used $H = U + PV = 5Nk_BT/2$.

$$\kappa_T = -\frac{1}{V}\left(\frac{\partial V}{\partial P}\right)_{T,N} = \frac{1}{P}, \quad \kappa_S = -\frac{1}{V}\left(\frac{\partial V}{\partial P}\right)_{S,N} = \frac{C_V}{C_P}\kappa_T = \frac{3}{5P} \tag{17}$$

and

$$\alpha_P = \frac{1}{V}\left(\frac{\partial V}{\partial T}\right)_{P,N} = \frac{1}{T} \tag{18}$$

It is easy to verify that the response functions results above satisfy the relation,

$$C_P = C_V + \frac{TV\alpha_P^2}{\kappa_T} \tag{19}$$

To use the micro-canonical ensemble we calculate the density of states $\Omega(E)$ directly. To calculate this, we note that the degeneracy comes from the number of available arrangements in the three phase space dimensions of each momentum. Since the KE is a sum of the squares of the momenta, we can consider spheres in a $3N$ dimensional space, where surfaces of these $3N$ dimensional spheres have constant values for the sum of the momenta squared. In three dimensions, the density of states on a surface is $4\pi p^2$. In n dimensions the density of states is $s_n = nc_n p^{n-1}$. (see e.g. Pathria and Beale - Appendix C), To find c_n, we can use a Gaussian integral trick as follows,

$$\int_{-\infty}^{\infty} \prod dx_i e^{-\sum_i x_i^2} = (\pi)^{n/2} = \int_0^{\infty} nc_n R^{n-1} e^{-R^2} DR = \frac{n}{2}C_n\Gamma(\frac{n}{2}) = (n/2)!C_n \tag{20}$$

so that $c_n = \pi^{n/2}/(n/2)!$ (Note that $\Gamma(n/2) = (n/2-1)!$). Using $s_n = nc_n R^{n-1}$ with $R \to p$ and $n = 3N$ gives,

$$s_{3N} = \frac{2\ \pi^{3N/2}}{(\frac{3N}{2}-1)!}p^{3N-1} \tag{21}$$

Applying the Gibb's correction $(1/N!)$, the phase space correction $(1/h^{3N})$, including the spatial contribution V^N, with $p^2 = 2mE$ gives the micro-canonical density of states,

$$\Omega(E) = \frac{2\pi^{1/2}V^N}{N!h^{3N}}\frac{(2\pi mE)^{3N/2-1/2}}{(\frac{3N}{2}-1)!} \tag{22}$$

Using Stirling's approximation and keeping the leading order terms gives the Sackur-Tetrode equation for the entropy of an ideal gas,

$$S = k_B ln(\Omega(E)) = Nk_B\left[ln[\frac{V}{N}\left(\frac{4\pi mU}{3Nh^2}\right)^{3/2}] + \frac{5}{2}\right] \tag{23}$$

The internal energy is then,

$$U = \frac{3h^2 N^{5/3}}{4\pi mV^{2/3}}Exp[\frac{2S}{3Nk_B} - \frac{5}{3}] \tag{24}$$

From (23) or (24) the other thermodynamic properties of interest can be calculated. Using the equipartition result it is easy to show that Eq. (23) and (12) are equivalent.

Finally we would like to find the grand canonical partition function. This can be calculated from the canonical partition function by summing over all numbers of particles as follows,

$$\Xi(T, V, \mu) = \sum_{N=1}^{\infty} z^N Z_N = \sum_{N=1}^{\infty} z^N \frac{\alpha^N}{N!} = e^{\alpha z} \tag{25}$$

where $z = e^{\beta\mu}$ is the fugacity, and $\alpha = V/\lambda^3$. We have,

$$\Phi_G = -PV = -k_B T ln(\Xi) = -k_B T \alpha e^{\beta\mu} \tag{26}$$

$$d\Phi_G = -SdT - PdV - Nd\mu = \left(\frac{\partial \Phi_G}{\partial T}\right)_{V,\mu} dT + \left(\frac{\partial \Phi}{\partial V}\right)_{T,\mu} dV + \left(\frac{\partial \Phi_G}{\partial \mu}\right)_{T,V} d\mu \tag{27}$$

Which again can be used to calculate all thermodynamic quantities, for example

$$-N = \left(\frac{\partial \Phi_G}{\partial \mu}\right)_{T,V} = -k_B T \beta \alpha e^{\beta\mu} = -\beta PV \tag{28}$$

which is the ideal gas law again (to find the last expression we used Eq. (26)).

C.   Quantum gases in a volume V: Grand canonical ensemble

The most basic problem in statistical mechanics of quantum systems is where we have a system with a known set of *single particle* energy levels. Given this set of energy levels, we would like to know the behavior of the system. There are many possible cases, including non-relativistic and relativistic problems in one, two and three dimensional boxes or some other sort of confining potential such as a harmonic potential. In solid state physics there is also the very general problem of single particle energy levels in periodic lattices, i.e. band structures. These single particle energy levels may be modified by adding spin and/or orbital degrees of freedom, and also the possibility of adding a magnetic field. Moreover these single particle solutions are the basis of self-consistent or mean field approaches such as Density functional theory and Nuclear Shell model calculations.

We start with the general problem of a set of single particle energy levels ϵ_l, where each energy level has degeneracy g_l. We use j to label the g_l degenerate levels, so that $j = 1...g_l$. Given this information, we would like to find the partition function for cases where classical, Bose and Fermi particles are placed into these energy levels. For the moment we concentrate on the case where the particles have no internal degrees of freedom, so for the Fermi particles, the occupancy of an energy level labelled by quantum numbers l, j, with ϵ_l can be either zero or one. For the Bose and classical cases however, any number of particles may be in each energy level. For the case of Fermi particles, we have,

$$\Xi_F = \sum_{n_1} ... \sum_{n_M} e^{-\beta \sum_{l=1}^{M} (\epsilon_l - \mu) n_l} = \prod_{l=1}^{M} \left(1 + e^{-\beta(\epsilon_l - \mu)}\right) = \prod_{l=1}^{M} \left(1 + z e^{-\beta\epsilon_l}\right) \tag{29}$$

where $z = e^{\beta\mu}$ and each sum is over the possiblities $n_l = 0, 1$ as required for Fermi statistics. For the case of Bose statistics the possibilities are $n_l = 0, 1, 2...\infty$ so we find

$$\Xi_B = \sum_{n_1} ... \sum_{n_M} e^{-\beta \sum_{l=1}^{M} (\epsilon_l - \mu) n_l} = \prod_{l=1}^{M} \left(\frac{1}{1 - e^{-\beta(\epsilon_l - \mu)}}\right) = \prod_{l=1}^{M} \left(\frac{1}{1 - z e^{-\beta\epsilon_l}}\right) \tag{30}$$

where the sums are carried out by using the formula for a geometric progression. The grand partition function for the Fermi and Bose cases are then given by,

$$\Phi_F = -PV = -k_B T ln(\Xi) = -k_B T \sum_{l=1}^{M} ln\left(1 + z e^{-\beta\epsilon_l}\right) \tag{31}$$

and

$$\Phi_B = -PV = -k_B T ln(\Xi) = k_B T \sum_{l=1}^{M} ln\left(1 - z e^{-\beta\epsilon_l}\right) \tag{32}$$

The average occupancy of each level is found by taking a partial derivative with respect to ϵ_l, so that,

$$< n_l >_F = -\frac{1}{\beta}\frac{\partial ln(\Xi)}{\partial \epsilon_l} = \frac{ze^{-\beta\epsilon_l}}{1 + ze^{-\beta\epsilon_l}} \tag{33}$$

and

$$< n_l >_B = -\frac{1}{\beta}\frac{\partial ln(\Xi)}{\partial \epsilon_l} = \frac{ze^{-\beta\epsilon_l}}{1 - ze^{-\beta\epsilon_l}} \tag{34}$$

The total number of particles in the system is then,

$$N = \sum_l < n_l > = z\frac{\partial ln(\Xi)}{\partial z} \tag{35}$$

A derivative with respect to β, while keeping z constant gives the internal energy,

$$U = -\frac{\partial ln(\Xi)}{\partial \beta} = \sum_l < n_l > \epsilon_l \tag{36}$$

To illustrate how this works, we carry through the calculations for non-relativistic ideal quantum gases, that we then compare with the ideal classical or Maxwell-Boltzmann gas described above.

D. Non-relativistic ideal quantum gases in a box with $V = L^3$

1. Energy levels and single particle density of states

The only additional input required to carry out calculations with the formulae (31)-(36) are the energy levels. To find the energy levels for a non-relativistic particle in a box, we consider a cubic box of volume $V = L^3$ with hard walls at $x = 0, L; y = 0, L; z = 0, L$ and solve the non-relativistic Schrodinger equation in the interior of the box. The wavefunction has to be zero at the boundaries, so we have,

$$\psi = A sin(k_x x) sin(k_y y) sin(k_z z), \tag{37}$$

with,

$$\epsilon_{k_x,k_y,k_z} = \frac{\hbar^2(k_x^2 + k_y^2 + k_z^2)}{2m}; \quad k_x = \frac{\pi n_x}{L}; \; k_y = \frac{\pi n_y}{L}; \; k_z = \frac{\pi n_z}{L}. \tag{38}$$

The solutions for one and two dimensional systems with hard walls are found by simply removing the k_y, k_z and k_z terms respectively. For a ultra-relativistic particle the energy is $\epsilon = pc = \hbar kc$, the same boundary conditions on $\vec{k}$ apply. As we shall see later, we often need to carry out a sum over all of the energy levels. To do this it is usually convenient to convert the sum to an integral,

$$\sum_{n_x,n_y,n_z} \rightarrow \left(\frac{L}{\pi}\right)^3 \int_0^\infty d^3k + T_0 = \left(\frac{L}{2\pi}\right)^3 \int_{-\infty}^\infty d^3k + T_0 \tag{39}$$

The last expression can also be found by solving the problem using a box with periodic boundary conditions using a wavefunction $e^{i\vec{k}\cdot\vec{r}}$, in which case $\vec{k} = 2\pi\vec{n}/L$, but n_x, n_y, n_z each take either positive or negative integers as well as zero. This analysis has to be taken with care in the case of Bosons where there is the possibility of a macroscopic density in the ground state. The term T_0 is added to take that possibility into account. The term T_0 in the Bose case is singular and needs to be treated separately, as discussed further in the particular cases that we study. It is essential to the analysis of Bose condensation.

It is often convenient to convert the integral $d^D k$ to an integral over a single variable (here D is the spatial dimension), either k, p or the energy $d\epsilon$. In the non-relativistic case, we have,

$$\int d^3k \rightarrow \int 4\pi k^2 dk \rightarrow \int \rho_3(\epsilon)d\epsilon \quad \text{with} \quad \rho_3(\epsilon) = 4(2)^{1/2}\pi\left(\frac{m}{\hbar}\right)^{3/2}\epsilon^{1/2} \tag{40}$$

Similar calculations in one and two dimensions yield,

$$\rho_1 = (2)^{1/2}\left(\frac{m}{\hbar}\right)^{-1/2}\frac{d\epsilon}{\epsilon^{1/2}}; \quad \rho_2 = 2\pi\frac{m}{\hbar^2}d\epsilon \tag{41}$$

Now that we have the energy levels and the single particle densities of states, we can find the thermodynamic behavior.

2. Thermodynamics properties of non-relativistic ideal quantum gases

Using the momentum as the integration variable and using $\vec{p} = \hbar \vec{k}$, from Eq. (29) we have,

$$ln(\Xi_F) = \sum_{n_x,n_y,n_z} ln\left(1 + ze^{-\beta p^2/2m}\right) = \left(\frac{L}{2\pi\hbar}\right)^3 \int_0^\infty dp\ 4\pi p^2 ln\left(1 + ze^{-\beta p^2/2m}\right) \tag{42}$$

so that

$$\Phi_F = -k_BT ln(\Xi_F) = -k_BT \left(\frac{L}{2\pi\hbar}\right)^3 \int_0^\infty dp\ 4\pi p^2 ln\left(1 + ze^{-\beta p^2/2m}\right) \tag{43}$$

and using $PV = k_BT ln(\Xi)$ we find,

$$\frac{P}{k_BT} = \frac{4\pi}{h^3} \int_0^\infty dp\ p^2 ln\left(1 + ze^{-\beta p^2/2m}\right); \quad \text{Fermi gas} \tag{44}$$

For the number of particles Eq. (35) yields,

$$\frac{N}{V} = \frac{4\pi}{h^3} \int_0^\infty dp\ p^2 \frac{ze^{-\beta p^2/2m}}{1 + ze^{-\beta p^2/2m}}; \quad \text{Fermi gas} \tag{45}$$

and Eq. (36) gives,

$$\frac{U}{V} = \frac{4\pi}{h^3} \int_0^\infty dp\ p^2 \frac{p^2}{2m} \frac{ze^{-\beta p^2/2m}}{1 + ze^{-\beta p^2/2m}}; \quad \text{Fermi gas} \tag{46}$$

The procedure for the Bose case has to take into account the possibility of Bose condensation

$$ln(\Xi_B) = -\sum_{n_x,n_y,n_z} ln\left(1 - ze^{-\beta p^2/2m}\right) = -\left(\frac{L}{2\pi\hbar}\right)^3 \int_0^\infty dp\ 4\pi p^2 ln\left(1 - ze^{-\beta p^2/2m}\right) - ln(1-z) \tag{47}$$

where the $ln(1-z)$ term on the right hand side takes into account the fact that in a Bose system the ground state can have macroscopic occupancy, as occurs in Bose condensation. We then have,

$$\Phi_B = k_BT \sum_{n_x,n_y,n_z} ln\left(1 - ze^{-\beta p^2/2m}\right) = k_BT \left(\frac{L}{2\pi\hbar}\right)^3 \int_0^\infty dp\ 4\pi p^2 ln\left(1 - ze^{-\beta p^2/2m}\right) + k_BT ln(1-z) \tag{48}$$

We thus separate the ground state term from the rest of the integral. Using $\Phi_G = -PV = -k_BT ln(\Xi)$ we find,

$$\frac{P}{k_BT} = -\frac{4\pi}{h^3} \int_0^\infty dp\ p^2 ln\left(1 - ze^{-\beta p^2/2m}\right) - \frac{1}{V} ln(1-z); \quad \text{Bose gas} \tag{49}$$

$$\frac{N}{V} = \frac{4\pi}{h^3} \int_0^\infty dp\ p^2 \frac{ze^{-\beta p^2/2m}}{1 - ze^{-\beta p^2/2m}} + \frac{1}{V} \frac{z}{1-z}; \quad \text{Bose gas} \tag{50}$$

and

$$\frac{U}{V} = \frac{4\pi}{h^3} \int_0^\infty dp\ p^2 \frac{p^2}{2m} \frac{ze^{-\beta p^2/2m}}{1 - ze^{-\beta p^2/2m}}; \quad \text{Bose gas} \tag{51}$$

Note that we dropped the additional term to account for the possibility of macroscopic occupancy of the ground state, as the $p^2/2m$ term goes to zero sufficiently quickly as $p \to 0$ that the ground state contribution can no longer be singular.

3. High and low temperature behavior of 3-d non-relativistic ideal Bose gas

The thermodynamic functions are most succinctly stated in terms of the functions $g_{3/2}(z)$ and $g_{5/2}(z)$ so that Eqs. (49) - (51) reduce to,

$$P = \frac{k_B T}{\lambda^3} g_{5/2}(z) - \frac{k_B T}{V} ln(1-z); \quad \frac{N}{V} = \frac{1}{\lambda^3} g_{3/2}(z) + \frac{1}{V} \frac{z}{1-z}; \quad \frac{U}{V} = \frac{3}{2} \frac{k_B T}{\lambda^3} g_{5/2}(z) \tag{52}$$

These expressions are found by making the substitution $x^2 = \beta p^2/2m$ and using the definition of the thermal de Broglie wavelength to write,

$$g_{5/2}(z) = -\frac{4}{\pi^{1/2}} \int dx \; x^2 ln(1 - ze^{-x^2}) = \sum_{l=1}^{\infty} \frac{z^l}{l^{5/2}}; \quad g_{3/2}(z) = z \frac{\partial}{\partial z} g_{5/2}(z) = \sum_{l=1}^{\infty} \frac{z^l}{l^{3/2}}. \tag{53}$$

The series expansion for $g_{5/2}$ is found by expanding the logarithm in the integral form of $g_{5/2}$ and then integrating the Gaussians that remain, using,

$$ln(1-y) = -\sum_{l=1}^{\infty} \frac{z^l}{l}; \quad \int_0^{\infty} dx \; x^2 e^{-lx^2} = \frac{\pi^{1/2}}{4} \frac{1}{l^{3/2}}. \tag{54}$$

The expansion for $g_{3/2}$ can be found by differention or by expanding $1/(1-y)$ and carrying out the Gaussian integrals. Note that if the term $ln(1-z)$ is negligible, then

$$U = \frac{3}{2} PV, \tag{55}$$

We shall see later that this is indeed the case. This relation also holds for the ideal classical gas and the Fermi gas, as we shall see later.

First we look at the behavior at high temperatures where we expect to recover the classical, Maxwell-Boltzmann gas. while the Bose case gives,

$$\frac{N}{V} = \frac{1}{\lambda^3} g_{3/2}(z) = \frac{1}{\lambda^3} (z + \frac{z^2}{2^{3/2}} + ..) \tag{56}$$

The only difference in these series is that the Fermi case alternates in sign and the Bose case does not. This is important if z is large, but is not important if z is small. At high temperatures λ is small, and so is N/V, so we expect z to be small. Keeping only the leading order term in the expansion above we have,

$$z = \frac{N\lambda^3}{V}; \quad \text{and using } \beta\mu = ln(z); \quad \mu = k_B T ln(\frac{N\lambda^3}{V}) \tag{57}$$

which is the same as the chemical potential found in the classical ideal gas (see Eq. (15)) of the lecture notes for Part 2. Note that the chemical potential is large and negative at high temperature, so the fugacity approaches zero. The fugacity is always positive as it is an exponential of real number.

From Eq. (52) using the leading order $g_{5/2} = z$, along with $z = N\lambda^3/V$ as found above, give the ideal gas law and the equipartition result for the internal energy of the classical ideal gas. Problem 4 of the assignment asks that you calculate the next correction to the classical limit. This is achieved by considering the next term in the expansion of the fugacity (56).

Now we consider the low temperature limit where Bose condensation can occur. As noted above, the chemical potential of gases are large and negative at high temperature, so the fugacity approaches zero as $T \to \infty$. At low temperatures, the chemical potential is dominated by the energy contribution. For a Bose system where the ground state energy is at zero energy, the change in energy on addition of a particle is zero, so the chemical potential approaches zero as $T \to 0$. In the Bose case, the equation for the number density of particles consists of a ground state part and a finite temperature part,

$$N = \frac{V}{\lambda^3} g_{3/2}(z) + \frac{z}{1-z} = N_1 + N_0 \tag{58}$$

where N_1 is the number of Bose particles in the excited states and N_0 is the number of Bose particles in the ground state. As noted above, the largest value that z can take for a Bose gas is $z = 1$, therefore the largest possible value that N_1 can take is,

$$N_1^{max} = \frac{V}{\lambda^3} g_{3/2}(1) = \frac{V}{\lambda^3} \zeta(3/2) \tag{59}$$

where $\zeta(x)$ is the Reimann zeta function and $\zeta(3/2) = 2.612....$ Bose condensation occurs when $N_1^{max} < N$ as if this occurs, the remaining Bose particles must be in the ground state. Therefore the condition for Bose condensation is,

$$N = N_1^{max} = \zeta(3/2)\frac{V}{\lambda_c^3}; \quad \text{or} \quad \frac{N\lambda^3}{V} = \frac{Nh^3}{V(2\pi mk_BT_c)^{3/2}} = \zeta(3/2) \tag{60}$$

or,

$$T_c = \frac{h^2}{2\pi mk_B}\left(\frac{N}{V\zeta(3/2)}\right)^{2/3}. \tag{61}$$

A high Bose condensation temperature is then favored by a high particle density (large N/V) of low mass (m) Bose particles. Using the mass and density of Helium 4 the above equation gives $T_c = 3.13K$. The superfluid transition in Helium 4 is actually at $T_c = 2.18K$ so the BEC theory is not good for Helium 4, but that is not surprising as Helium 4 is not an ideal gas. Later we shall discuss atom traps where BEC is a much better model.

Because $\mu = 0$ and hence $z = 1$ in the Bose condensed state, the thermodynamics can be calculated in terms of ζ functions, for example the fraction of the Bose gas that is in the condensed phase is,

$$f_s = \frac{N_0}{N} = 1 - \frac{N_1}{N} = 1 - \frac{V}{N\lambda^3}\zeta(3/2) = 1 - \left(\frac{T}{T_c}\right)^{3/2} \qquad T \leq T_c. \tag{62}$$

where f_s is the condensed or superfluid fraction of the gas. The internal energy is given by,

$$\frac{U}{V} = \frac{3}{2}\frac{k_BT}{\lambda^3}g_{5/2}(1) = \frac{3}{2}\frac{k_B(2\pi mk_B)^{3/2}}{h^3}T^{5/2}g_{5/2}(1) = \frac{3}{2}\frac{N}{V}k_BT\left(\frac{T}{T_c}\right)^{3/2}\frac{g_{5/2}(1)}{g_{3/2}(1)} \qquad T \leq T_c \tag{63}$$

The specific heat at constant volume is then (using $\zeta(5/2) = 1.3415$,

$$C_V = \frac{15}{4}\frac{k_B(2\pi mk_B)^{3/2}}{h^3}T^{3/2}g_{5/2}(1) = \frac{15}{4}Nk_B\left(\frac{T}{T_c}\right)^{3/2}\frac{g_{5/2}(1)}{g_{3/2}(1)} \tag{64}$$

The specific heat then goes to zero as $T \to 0$. The peak value of the specific heat is at $T = T_c$, where it takes the value

$$C_V(T_c) = \frac{15}{4}Nk_B\frac{g_{5/2}(1)}{g_{3/2}(1)} \approx 1.926Nk_B \tag{65}$$

This can be compared to the ideal gas result $C_v = 1.5Nk_B$ (Dulong-Petit law), which is correct at high temperature. There is a cusp in the specific heat at $T = T_c$ due to the Bose condensation phase transition. This cusp behavior is quite different that that observed in Helium 4 (the λ transition) where there is a much sharper divergence at the transition, so the specific heat measurment clearly shows that the ideal Bose gas is a poor model for superfluid Helium. Finally, using $PV = 2U/3$, we have,

$$PV = Nk_BT\left(\frac{T}{T_c}\right)^{3/2}\frac{g_{5/2}(1)}{g_{3/2}(1)} \qquad T \leq T_c \tag{66}$$

In the condensed phase, the pressure is then smaller than that of the ideal classical gas. In writing this expression, we have ignored the term $ln(1-z)$, moreover in doing the calculation of N we have also avoided discussing the term $z/(1-z)$, that is singular as $z \to 1$. We now discuss these terms. In order to discuss these terms, we have to consider a finite system, so that z is not exactly one, but instead approaches 1 with increasing volume. The dependence of z on volume can be deduced from Eq. (62), so that in the condensed phase we define $z = 1 - \delta$, where δ is small so that,

$$\frac{z}{N(1-z)} \approx \frac{1}{N\delta} = 1 - \frac{V}{N\lambda^3}\zeta(3/2) = f_s, \quad \text{so that} \quad \delta = \frac{1}{Nf_s} \tag{67}$$

so the fugacity approaches zero as $1/N$, provided $f_s > 0$. From this result it is evident that the term

$$ln(1-z) = ln(\frac{1}{Nf_s}) \approx -ln(Nf_s). \tag{68}$$

In the equation $P = k_B T g_{5/2}(z)/\lambda^3 - ln(1-z)/V$ (see Eq. (52)), the first term is of order one, however the second term goes to zero rapidly as $|ln(Nf_s)| << V$ and is negligible in comparison to terms of order one. We are thus justified in ignoring it in the evaluation of the equation of state, for example in Eqs. (49) and (52). In a similar way the corrections to the thermodynamics of the BEC phase due to deviations of z from one are of order $1/N$ compared to the leading order terms, so they can be neglected. In the thermodynamic limit the results give above for the equation of state, f_s and C_V are *exact* in the condensate phase.

If we carry through the analysis for the ideal Bose gas in two dimensions, the key difference is that the function $g_{3/2}(z)$ is changed to $g_1(z)$ and this function diverges as $z \to 1$. The fraction of the gas particles that go into the condensate is then finite for all $T > 0$ so there is no finite temperature BEC phase transition in the ideal Bose gas.

4. Non-relativistic Fermi gas in 3-d at low and high temperature

We start with Eq. (44) and use the same change of variables as used in Bose case, $x^2 = \beta p^2/2m$, and we define,

$$f_{5/2}(z) = \frac{4}{\pi^{1/2}} \int dx \, x^2 ln(1 + ze^{-x^2}) = \sum_{l=1}^{\infty} \frac{(-1)^{l+1}z^l}{l^{5/2}}; \qquad f_{3/2}(z) = z\frac{\partial}{\partial z}f_{5/2}(z) = \sum_{l=1}^{\infty} \frac{(-1)^{l+1}z^l}{l^{3/2}} \qquad (69)$$

so that the thermodynamics of the Fermi gas is found from equations that look very similar to those of the Bose case,

$$P = \frac{k_B T}{\lambda^3}f_{5/2}(z); \qquad \frac{N}{V} = \frac{1}{\lambda^3}f_{3/2}(z); \qquad \frac{U}{V} = \frac{3}{2}\frac{k_B T}{\lambda^3}f_{5/2}(z) \qquad (70)$$

In the high temperature limit $z \to 0$ ($T \to \infty, \mu \to -\infty, \beta\mu \to -\infty$), Fermi case is,

$$\frac{N}{V} = \frac{1}{\lambda^3}f_{3/2}(z) = \frac{1}{\lambda^3}(z - \frac{z^2}{2^{3/2}} + ..) \qquad (71)$$

To leading order this gives the same result as the Bose case, though the next order correction is different. The Fermi gas has higher pressure than the Bose or classical cases and this is seen in the next to leading order expansion at high temperatures.

The behavior of the Fermi gas at low temperatures is very different than that of the Bose or the classical gas, due to the fact that the maximum number of particles that can occupy an energy level is one for Fermions. As particles are added into the box they must occupy higher and higher energy levels, so that the last particles to be added are in states with high kinetic energy. Even at low temperatures the Fermi gas then has a high pressure, called the degeneracy pressure, and the particles have high kinetic energy. This is the mechanism by which white dwarf stars maintain stability, i.e. the degeneracy pressure of the electrons balances the gravitational collapse pressure. As the mass of the star gets larger the degeneracy pressure of the electrons is not large enough and the electrons combine with the protons to form neutrons. The neutron degeneracy pressure is larger than that of the electrons and enables stability for higher mass stars. For larger enough mass however, even the neutron degeneracy pressure is not sufficient and a black hole is formed. However to analyse these cases we need to treat the relativistic case, whereas here we are treating the non-relativistic problem which applies to many problems in atomic and solid state physics.

To understand the degeneracy pressure and other properties of ideal Fermi gases, we first need to understand the chemical potential and the fugacity at low temperatures. Since at low temperatures the chemical potential is controlled by the energy contribution, and the energy required to add a particle to the volume is the lowest unoccupied single particle energy level, the chemical potential is finite and positive at low temparutures. In that case, $\beta\mu$ becomes large at low temperature and the fugacity is then very large and positive. The series expansions in Eq. (69) for $f_{3/2}$ and $f_{5/2}$ are poorly convergent at low temperatures, so we need a different approach. Following Somerfeld, it is more convenient to carry out an expansion in $\nu = \beta\mu = ln(z)$. The procedure is as follows. We work the the integral form of $f_{3/2}(z)$,

$$f_{3/2}(z) = \frac{4}{\pi^{1/2}} \int_0^{\infty} dx \, x^2 \frac{ze^{-x^2}}{1 + ze^{-x^2}} \qquad (72)$$

We change variables to $y = x^2$, then and integrate by parts to find,

$$f_{3/2}(z) = \frac{2}{\pi^{1/2}} \int_0^{\infty} dy \frac{y^{1/2}}{e^{y-\nu} + 1} = \frac{4}{3\pi^{1/2}} \int_0^{\infty} dy \frac{y^{3/2}e^{y-\nu}}{(e^{y-\nu} + 1)^2} \qquad (73)$$

The integration by parts leads to an integrand that is cnvergent at large y. Now we expand $y^{3/2}$ in a Taylor series about ν,

$$y^{3/2} = (\nu + (y-\nu))^{3/2} = \nu^{3/2} + \frac{3}{2}\nu^{1/2}(y-\nu) + \frac{3}{8}\nu^{-1/2}(y-\nu)^2 + ... \tag{74}$$

so that,

$$f_{3/2}(z) = \frac{4}{3\pi^{1/2}} \int_0^\infty dy \frac{e^{y-\nu}}{(e^{y-\nu}+1)^2}(\nu^{3/2} + \frac{3}{2}\nu^{1/2}(y-\nu) + \frac{3}{8}\nu^{-1/2}(y-\nu)^2 + ...). \tag{75}$$

Defining $t = y - \nu$ yields,

$$f_{3/2}(z) = \frac{4}{3\pi^{1/2}} \int_{-\nu}^\infty dt \frac{e^t}{(e^t+1)^2}(\nu^{3/2} + \frac{3}{2}\nu^{1/2}t + \frac{3}{8}\nu^{-1/2}t^2 + ...) \tag{76}$$

Now we break the integral up as,

$$\int_{-\nu}^\infty = \int_{-\infty}^\infty - \int_{-\infty}^{-\nu} \tag{77}$$

where the second integral is exponentially small, ie. $O(e^{-\nu})$, so we can ignore it. Finally we have,

$$f_{3/2}(z) = \frac{4}{3\pi^{1/2}}(\nu^{3/2}I_0 + \frac{3}{2}\nu^{1/2}I_1 + \frac{3}{8}\nu^{-1/2}I_2 + ...); \quad \text{where} \quad I_n = \int_{-\infty}^\infty dt \frac{t^n e^t}{(e^t+1)^2} \tag{78}$$

$I_0 = 1$, while by symmetry I_n is zero for odd n. For even $n > 0$, I_n is related to the Reimann zeta function, through,

$$I_n = 2n(1 - 2^{1-n})(n-1)!\zeta(n), \quad \text{with} \quad \zeta(2) = \frac{\pi^2}{6}, \quad \zeta(4) = \frac{\pi^4}{90}, \quad \zeta(6) = \frac{\pi^6}{945} \tag{79}$$

At very low temperatures, we take only the leading order term in the expansion so that,

$$\frac{N}{V} = \frac{1}{\lambda^3} \frac{4}{3\pi^{1/2}}(\beta\mu_0)^{3/2} I_0 \tag{80}$$

where μ_0 is the leading order expression for the chemical potential at low temperatures. Solving yields,

$$\mu_0 = \epsilon_F = \frac{\hbar^2}{2m}\left(\frac{6\pi^2 N}{V}\right)^{2/3} \tag{81}$$

The fermi energy is calculated directly using,

$$\epsilon_F = \hbar^2 k_F^2/2m; \quad \text{with} \quad N = \left(\frac{L}{2\pi}\right)^3 \int_0^{k_F} 4\pi k^2 dk \tag{82}$$

that of course leads to the same result. However the Sommerfeld method enables us to also calculate the temperature dependence. To find the first temperature dependent term, we take the next term in the expansion of the chemical potential.

$$\frac{N}{V} = \frac{1}{\lambda^3} \frac{4}{3\pi^{1/2}}[(\beta\mu)^{3/2} I_0 + \frac{3}{8}(\beta\mu)^{-1/2} I_2 + ...] \tag{83}$$

We define μ_1 to be the next to leading estimate of μ and using $I_2 = \pi^2/3$, find that it is given by,

$$\frac{N}{V} = \frac{1}{\lambda^3} \frac{4}{3\pi^{1/2}}[(\beta\mu_1)^{3/2} + \frac{3}{8}\frac{\pi^2}{6}(\beta\mu_0)^{-1/2}]. \tag{84}$$

which may be written as,

$$(\beta\mu_0)^{3/2} = (\beta\mu_1)^{3/2} + \frac{\pi^2}{8}(\beta\mu_0)^{-1/2} \quad \text{or} \quad (\beta\mu_1)^{3/2} = (\beta\mu_0)^{3/2}[1 - \frac{\pi^2}{8}(\beta\mu_0)^{-2}] \tag{85}$$

Solving and using $\beta\mu_0 = \beta\epsilon_F$ gives,

$$\mu_1 = \epsilon_F[1 - \frac{\pi^2}{8}\left(\frac{k_BT}{\epsilon_F}\right)^2]^{\frac{2}{3}} = \epsilon_F[1 - \frac{\pi^2}{12}\left(\frac{k_BT}{\epsilon_F}\right)^2 + O(\left(\frac{k_BT}{\epsilon_F}\right)^4]$$ (86)

It is not too difficult to calculate the next term in the expansion of μ,

$$\mu_2 = \epsilon_F[1 - \frac{\pi^2}{12}\left(\frac{k_BT}{\epsilon_F}\right)^2 - \frac{\pi^4}{80}\left(\frac{k_BT}{\epsilon_F}\right)^4 + O(\left(\frac{k_BT}{\epsilon_F}\right)^6)]$$ (87)

It is then evident that this is a rapidly convergent series for all $kT < \epsilon_F$. For many applications this is well satisfied so the low temperature thermodynamics is deduced from this form of the chemical potential. To find the thermodynamics, we also need an asymptotic expansion for $f_{5/2}(z)$ (see e.g. Pathria and Beale p 236),

$$f_{5/2}(\nu) = \frac{8}{15\pi^{1/2}}(\nu^{5/2} + \frac{5\pi^2}{8}\nu^{1/2} + ...) = \frac{8}{15\pi^{1/2}}\nu^{5/2}(1 + \frac{5\pi^2}{8}\nu^{-2} + ...)$$ (88)

From Eq. (70) to leading order in the temperature we write,

$$U = \frac{3k_BTV}{2\lambda^3}\frac{8}{15\pi^{1/2}}(\beta\mu_1)^{5/2}(1 + \frac{5\pi^2}{8}(\beta\mu_0)^{-2}) = \frac{3k_BTV}{2\lambda^3}\frac{8(\beta\mu_0)^{5/2}}{15\pi^{1/2}}[(1 - \frac{5\pi^2}{24}(\beta\mu_0)^{-2})](1 + \frac{5\pi^2}{8}(\beta\mu_0)^{-2})$$ (89)

Using a leading order expansion and some work on the prefactor we find,

$$U = \frac{3}{5}N\epsilon_F[1 + \frac{5}{12}\pi^2\left(\frac{k_BT}{\epsilon_F}\right)^2]$$ (90)

The specific heat is then,

$$\frac{C_V}{Nk_B} = \frac{\pi^2}{2}\frac{k_BT}{\epsilon_F}$$ (91)

and the equation of state is,

$$PV = \frac{2}{3}U = \frac{2}{5}N\epsilon_F[1 + \frac{5}{12}\pi^2\left(\frac{k_bT}{\epsilon_F}\right)^2]$$ (92)

Note that at the densities typical of metals, and at room temperature, the electrons at the Fermi energy have velocities characteristic of a classical gas with temperatures roughly $10,000K$. This is due to the pecular nature of the exchange interaction, or Pauli principle. For this reason high density Fermi systems become more ideal as their density increases as in that limit, the exchange interaction dominates.

The Fermi factor is the average number of particles in each energy level,

$$<n_p> = \frac{1}{exp\beta(\epsilon - \mu)) + 1}$$ (93)

At low temperatures, this function approaches a step function, where states below the Fermi energy, $\epsilon_p < \epsilon_F$, are fully occupied, while those above the Fermi energy are unoccupied. The width of the step function is given by k_BT/ϵ_F. We shall return to this issue when we look at applications of Fermi and Bose Gases.

E.   Spin half paramagnets and Ising ferromagnets

The study of spin half magnets have played a key role in statistical physics, particularly in developing an understanding of phase transitions. Ising in his PhD thesis showed that the one dimensional Ising magnet does not have a phase transition at finite temperature while Onsager in a beautiful piece of work proved that the Ising model in two dimensions does have a phase transition. Ferromagnets are materials that exhibit spontaneous symmetry breaking where at low temperatures magnetization spontaneously appears without the application of an external field. In contrast paramagnets require an applied field in order to exhibit magnetization and at low field, h, the magnetization, m is proportional to the applied field. We analyse simple examples of a spin half paramagnet and a spin half ferromagnet.

1. Spin half paramagnet

We consider a case where the applied field lies along the easy axis of a magnet, so that the Hamiltonian is,

$$H = -\mu_s h \sum_i S_i \tag{94}$$

where μ_s is the magnetic moment of the system, h is the applied field and $S = \pm 1$ is the spin. The statistical mechanics is easy to carry through as follows,

$$Z = \prod_i^N (\sum_{S_i \pm 1} e^{\beta \mu_s h S_i}) = 2^N Cosh^N(\beta \mu_s h) \tag{95}$$

The magnetization is given by,

$$m = \frac{\mu_s}{N} \sum_i < S_i > = \frac{\mu_s}{N} \frac{\partial(ln(Z))}{\partial(\beta h)} = \mu_s tanh(\beta \mu_s h) \tag{96}$$

At low fields, we can expand $tanh(x) = x - x^3/3$, so that $m = \beta \mu_s^2 h$. A second important measurable quantity is the magnetic susceptibility,

$$\chi = \frac{\partial m}{\partial h} = \beta \mu_s^2 sech^2(\beta \mu h) \to \frac{\mu_s^2}{k_B T}, \ as \ h \to 0 \tag{97}$$

the property $\chi \propto 1/T$ is called the Curie law and is used in many experiments to extract the value of μ_s for a material.

2. Infinite range model of an Ising ferromagnet

The Ising model is very difficult, even in two dimensions where there is an exact solution. However the infinite range model is relatively easy to solve and exhibits an interesting phase transition. The infinite range model is often the same as a mean field model, as is the case for the Ising ferromagnet. Mean field theory in its many forms, and with many different names, is the most important first approach to solving complex interacting many body problems. The Hamiltonian for the infinite range model is,

$$H = -\frac{J}{N} \sum S_i S_j \tag{98}$$

so the partition function is,

$$Z = (\prod_i^N \sum_{S_i \pm 1}) e^{\beta \frac{J}{N} \sum_{ij} S_i S_j} = (\prod_i^N \sum_{S_i \pm 1}) e^{\beta \frac{J}{N} (\sum_i S_i)^2} \tag{99}$$

Using the Gaussian integral,

$$\int_{-\infty}^{\infty} e^{-x^2 + bx} dx = \frac{\sqrt{\pi}}{\sqrt{a}} e^{b^2/4a} \tag{100}$$

we write,

$$Z = \int_{-\infty}^{\infty} \frac{dx}{\sqrt{\pi}} e^{-x^2} \prod_i^N (\sum_{S_i \pm 1} e^{2x(\beta \frac{J}{N})^{1/2} S_i}) \tag{101}$$

Doing the sums gives,

$$Z = \int_{-\infty}^{\infty} \frac{dx}{\sqrt{\pi}} e^{-x^2} 2^N [Cosh(2x(\beta \frac{J}{N})^{1/2})]^N \tag{102}$$

We write this in the form,

$$Z = \int_{-\infty}^{\infty} \frac{dx}{\sqrt{\pi}} e^{f(x)}; \quad where, \quad f(x) = -x^2 + N[ln(2) + ln(Cosh(2x(\beta\frac{J}{N})^{1/2})] \tag{103}$$

Since $f(x)$ contains a large parameter N, it is a sharply peaked function, so we can use the method of steepest descents. This method states that if the function $f(x)$ has a set of maxima, then the integral is dominated by the largest of these maxima, in the thermodynamic limit. At the dominant maximum, x_{max}, the first derivative is zero, so the expansion to quadratic order is,

$$f(x) = f(x_{max}) - \frac{(x - x_{max})^2}{2!}|f''(x_{max})| + ... \tag{104}$$

where $f''(x_{max}) < 0$ as we are at a maximum. Using this expansion in the integral we find,

$$\int e^{f(x)} dx \rightarrow e^{f(x_{max})} \int_{-\infty}^{\infty} e^{-\frac{(x - x_{max})^2}{2!} f''(x_{max})} dx = \left(\frac{2\pi}{|f''(x_{max})|}\right)^{1/2} e^{f(x_{max})}. \tag{105}$$

The problem then reduces to finding the maxima of the function $f(x)$, or the minima of the function $-f(x)$. To find the maxima in the case of the Ising model, we take a derivative with respect to x of $f(x)$ in Eq. (103), that leads to,

$$x = N(\frac{\beta J}{N})^{1/2} tanh(2\frac{\beta J}{N})^{1/2} x \tag{106}$$

We define, $y = 2(\beta J/N)^{1/2}x$ to find,

$$y = 2\beta J tanh(y) \tag{107}$$

For small values of $\beta J < (\beta J)_c$, the only solution to this equation is at $y = 0$, so in that case,

$$Z \rightarrow \left(\frac{\pi}{|f''(x_{max})|}\right)^{1/2} \frac{1}{\sqrt{\pi}} e^{Nln(2)} \tag{108}$$

The Helmholtz free energy is, $F = -k_B T N ln(2)$, where we drop the prefactor terms that are much lower order. For large values of $\beta J > (\beta J)_c$, there are three solutions. The behavior in this regime can be treated analytically by expanding to cubic order in y, so that,

$$y = 2\beta J(y - \frac{1}{3}y^3) \tag{109}$$

this has three solutions,

$$y = 0; \quad y = \pm[3(2\beta J - 1)]^{1/2} \tag{110}$$

When $2\beta J > 1$, the second pair of solutions is real, while when $2\beta J < 1$ they are imaginary. The critical point is then at $(\beta J)_c = \frac{1}{2}$, and the behavior near the critical point is $y \approx [6(\beta J - (\beta J)_c)]^{1/2}$.

Integration of Eq. (109) or a fourth order expansion of (103) leads to,

$$-f_R(y) \approx a_1(T - T_c)y^2 + a_2 y^4, \tag{111}$$

where a_1 and a_2 are positive and constant terms along with higher order terms in y have been dropped. This expression is the same as the Landau free energy for an Ising system, as we shall see in the next section of the course. The function $f(y)$ is a reduced free energy. We then interpet y as the order parameter for the Ising model, so that $y \propto m$, and we find that the order parameter approaches zero as $m \propto (T_c - T)^{1/2}$ which is typical mean field behavior.

3. Spin half nearest neighbor Ising model in one dimension

The one-dimensional nearest neighbor Ising model has Hamiltonian,

$$H = -J \sum_{i=1}^{N} S_i S_{i+1} \tag{112}$$

where $S_i = \pm 1$. We will use periodic boundary conditions so the model is defined on a ring. It is useful to solve this problem using transfer matrices as they can be generalized to many problems and provide a method for tranforming a classical problem at finite temperature into the ground state of a quantum problem in one lower dimensions. The transfer matrix for the one dimensional Ising model is a two by two matrix, with matrix elements,

$$T_{S,S'} = e^{\beta J S S'} \tag{113}$$

where S, S' take values ± 1 as usual. The partition function may then be written as,

$$Z = \sum_{S_1}\sum_{S_2}....\sum_{S_N} e^{\beta J \sum_i S_i S_{i+1}} = \sum_{S_1}\sum_{S_2}....\sum_{S_N} < S_1|\hat{T}|S_2 >< S_2|\hat{T}|S_3 > .... < S_N|\hat{T}|S_1 > \tag{114}$$

This reduces to,

$$Z = tr(T^N) = \lambda_1^N + \lambda_2^N \tag{115}$$

where $\lambda_{1,2}$ are the eigenvalues of the transfer matrix T. The problem is then reduced to diagonalizing a two by two matrix. For the one-dimensional Ising model, we define $\alpha = e^{\beta J}$
and find that the eigenvalues of the transfer matrix are,

$$\lambda_1 = 2Cosh(\beta J); \qquad \lambda_2 = 2Sinh(\beta J) \tag{116}$$

so that,

$$Z = 2^N[Cosh^N(\beta J) + Sinh^N(\beta J)] \tag{117}$$

The specific heat can be calculated by using,

$$F = -k_B T ln(Z) - k_B T N[ln(2) + ln(Cosh(\beta J))] \tag{118}$$

so that,

$$C_V = T\frac{\partial^2 F}{\partial T^2} = Nk_B(\frac{J}{k_B T})^2 sech^2(\frac{J}{k_B T}) \tag{119}$$

At low temperatures this reduces to,

$$\frac{C_V}{Nk_B} \approx (\frac{J}{k_B T})^2 Exp[-\frac{2J}{k_B T}] \qquad as \quad T \to 0 \tag{120}$$

while

$$\frac{C_V}{Nk_B} \approx (\frac{J}{k_B T})^2 \qquad as \quad T \to \infty \tag{121}$$

The specific heat thus approaches zero exponentially at low temperatures and approaches zero algebraically at high temperatures. There is a peak in the specific heat at around $J = k_B T$. This is typical of systems that have a "gap" of order J between the ground state and the first excited state.

Solution of the two dimensional Ising model is carried out using the transfer matrix method, however the transfer matrix is of dimension $2^L \times 2^L$ where L is the transverse dimension of the square lattice strip. In a spectacular calculation, Onsager found the exact solution and from it found the following results (1944),

$$(\beta J)_c = \frac{1}{2}ln(1 + \sqrt{2}) \qquad or \qquad (\frac{k_B T}{J})_c \approx 2.2691... \tag{122}$$

and near the critical point the specific heat behaves as, for $T < T_c$,

$$\frac{C_V}{Nk_B} \approx \frac{2}{\pi}(\frac{2J}{k_B T_C})^2[-ln(1 - \frac{T}{T_c}) + ln(\frac{k_B T}{2J}) - (1 + \frac{\pi}{4})] \tag{123}$$

The specific heat thus diverges logarithmically on approach to T_c. The low and high temperature behavior is similar to that in the one dimensional case.

The magnetization can also be calculated. In the one dimensional case the transfer matrix can be extended to treat the hamiltonian,

$$H = -J \sum_i S_i S_{i+1} - h \sum_i S_i \tag{124}$$

The magnetization is found from $\partial ln(Z)/\partial(h)$, leading to,

$$m(h,T) = \frac{Sinh(\beta h)}{[Sinh^2(\beta h) + e^{-4\beta J}]^{1/2}}; \qquad 1d\ Ising. \tag{125}$$

From this expression it is seen that the magnetization is zero for $h = 0$ in one dimension. Note however that the susceptibility $\chi = \partial m/\partial h$ is not zero even in one dimension, and in fact is large as $T \to 0$.

In two dimensions an exact result in finite field has not been found, but the magnetization in zero field has been found, with the result that for $T < T_c$ with $h = 0$,

$$m(h = 0, T) = \left(1 - [Sinh(2\beta J)]^{-4}\right)^{1/8} \qquad 2d\ Ising,\ \ T < T_c \tag{126}$$

Near the critical point this reduces to,

$$m(h = 0, T) \propto (T_c - T)^{1/8} \qquad T < T_c,\ h = 0 \tag{127}$$

The critical exponent for the Ising order parameter is thus $1/8$ in two dimensions and $1/2$ in infinite dimensions (mean field theory). There is no phase transition in one dimension. What is the behavior in three dimensions?? We shall return to the general issue of phase transitions and critical exponents in Part 3 of the course.

II. PHOTONS AND PHONONS

A. Blackbody spectrum and photon gas thermodynamics

One of the the most remarkable predictions of quantum statistical physics is the Planck blackbody spectrum. Planck derived this prior to the development of the Bose gas theory that we discussed above, however it is just a special case of that theory. To find the blackbody spectrum we consider the energy levels of a particle in a box, though now the particle is a photon, so it has the energy-momentum dispersion relation $\epsilon_p = pc = \hbar kc = \hbar\omega = h\nu = hc/\lambda_\nu$. This is an ultrarelativistic case. Only the magnitude of the momentum appears in the energy-momentum relation, so we can use the same analysis that we carried out for the non-relativistic Bose gas, but with the replacement $\epsilon_p = pc$, where c is the velocity of light. Moreover, we set the chemical potential to zero as there can be an infinity of photons at zero energy. Actually the chemical potential of photons is not always zero as there are cases in photochemistry and photovoltaics where photons have a chemical potential that is less than zero. However for the case of photons in a box, i.e. blackbody radiation, the chemical potential is zero. We are thus considering the Bose condensed phase of the photon gas. However we are only interested in the excited state part of the system.

Applying the ideal Bose gas theory with $\epsilon_p = pc$ and $\mu = 0$ so that $z = 1$ for the photon case, we find,

$$ln(\Xi) = -2 \left(\frac{L}{2\pi\hbar}\right)^3 \int_0^\infty 4\pi p^2 dp\ ln(1 - e^{-\beta pc}), \tag{128}$$

while the number of excited state photons is,

$$N = 2 \left(\frac{L}{2\pi\hbar}\right)^3 \int_0^\infty 4\pi p^2 dp\ \frac{e^{-\beta pc}}{1 - e^{-\beta pc}} = V \int d\omega\ n(\omega) \tag{129}$$

and the internal energy is given by,

$$U = 2 \left(\frac{L}{2\pi\hbar}\right)^3 \int_0^\infty 4\pi p^2 dp\ (pc) \frac{e^{-\beta pc}}{1 - e^{-\beta pc}} = V \int d\omega\ u(\omega) \tag{130}$$

where $n(\omega)$ is the number density of photons and $u(\omega)$ is the energy density at angular frequency ω. Notice that the additional terms, $ln(1 - z)$ that is usually in the equation for $ln(\Xi)$ and the term $z/(1 - z)$ that is usually in the

equation for N are omitted. The additional factor of two in front of these equations is due to the two polarizations that are possible for the photons. Using $p = \hbar\omega/c$, we find,

$$n(\omega) = \frac{1}{\pi^2 c^3} \frac{\omega^2}{e^{\beta\hbar\omega} - 1}; \qquad u(\omega) = \frac{\hbar}{\pi^2 c^3} \frac{\omega^3}{e^{\beta\hbar\omega} - 1} \tag{131}$$

These functions characterize the "blackbody spectrum" with temperature T.

The thermodynamics is found by integration, using the integral,

$$\int_0^\infty \frac{x^{s-1} dx}{e^x - 1} = \Gamma(s)\zeta(s), \tag{132}$$

where $\Gamma(s) = (s-1)!$ for s a positive integer , and $\zeta(3) = 1.202...$, $\zeta(4) = \pi^4/90$. For $s = 4$, we find $\gamma(s)\zeta(s) = \pi^4/15$.

$$\frac{U}{V} = \frac{\pi^2 k_B^4}{15\hbar^3 c^3} T^4; \quad PV = \frac{1}{3}U; \quad N = V\frac{2\zeta(3)(k_B T)^3}{\pi^2 \hbar^3 c^3} \tag{133}$$

Two other nice relations for the photon gas that can be derived from standard thermodynamic relations are $S = 4U/(3T)$, $C_V = 3S$.

The Stefan-Boltzmann law $I_{SB} = \sigma T^4$, is the power per unit area radiated from a blackbody with emissivity one. The relation I_{SB} and U/V of the photon gas is, are as follows,

$$I_{SB}(T) = \frac{c}{4}\frac{U}{V} = \sigma_{SB}T^4; \quad \text{where} \quad \sigma_{SB} = \frac{\pi^2 k_B^4}{60\hbar^3 c^2} \tag{134}$$

where σ_{SB} is the Stefan Boltzmann constant. The factor $c/4$ has two orgins, the first factor (c) comes from the relationship between the energy of a travelling wave and its intensity, and the second is a geometric factor due to an assumption of isotropic emission from a small surface element on the surface of the emitter. To understand the first factor, consider a classical EM wave in free space with energy density $u = \epsilon_0 E_0^2/2 +_0^2/(2\mu_0)$. In the direction of propagation of the wave, the energy crossing a surface of area A per unit time is,

$$Energy\ per\ unit\ time = Power = u * A * c \quad \text{so that} \quad I_w = Power/Area = uc \tag{135}$$

where I_w is the intensity of the wave. This applies to both the peak and rms intensity of the wave, provided the energy density is the peak or rms value respectively. The geometric factor comes from considering a small flat surface element that emits radiation in all directions. In the case of blackbody radiation, this element is considered to be at the surface, so it emits half of its radiation back into the black body and half out of the black body. In addition, the radiation in the direction normal to the surface is reduced from the total radiation emitted from the surface element due to the assumption of isotropic emission. The component normal to the surface is found by finding the component of the electric field in the formal direction, $E_0 cos(\theta)$, then squaring this to get the correct projection of the intensity, and then averaging over angles θ in a hemisphere. The result is that we need to average $cos^2(\theta)$ over a half period. This leads to a geometric factor of $1/2$. Multiplying these two factors of $1/2$ gives the total geometric factor of $1/4$. In most applications, the Stefan-Boltzmann law needs to be modified to account for the emissivity of the material (e) and the geometry of the surface and the location of the observer with respect to the surface, if the surface is not spherical.

The Planck radiation law is often quoted in a slightly different way. It is often defined to be the radiant spectral intensity per unit solid angle, which is related to the spectral energy density by $u(\omega)$ by $i_s(\omega, T) = c\,u(\omega)/(4\pi)$, where 4π is solid angle of a sphere. Moreover, various forms of i_s are common, including:

$$i_s(\omega, T) = \frac{\hbar}{4\pi^3 c^2}\frac{\omega^3}{e^{\beta\hbar\omega} - 1} \quad \text{or} \quad i_s(\nu, T) = \frac{2h}{c^2}\frac{\nu^3}{e^{\beta h\nu} - 1}; \quad \text{or} \quad i_s(\nu, T) = \frac{2c^2 h}{\lambda^5}\frac{1}{e^{\beta hc/\lambda} - 1} \tag{136}$$

The blackbody spectrum provides a surprisingly good description of the cosmic microwave background, with temperature $T_{CMB} = 2.713K$. It also describes the spectrum of stars very well, with some examples being: Our Sun with $T = 5800K$, Antares with $T = 3400K$, Spica with $T = 23,000K$. In fact one of the quantities that is measured for a new star is its luminosity. In Astronomy the bolometric luminosity is the total luminosity while the luminosity is the visible part of the radiant energy. The bolometric luminosity, L, is equal to the emitted power, and from the Stefan-Boltzmann law we find,

$$L = 4\pi R^2 e\sigma T^4 \tag{137}$$

For main sequence stars there is also a relation between the mass of a star and the luminosity $L \propto M^{3.9}$. In these stars, the tendency toward gravitational collapse is balanced by the radiation pressure of the photons that are generated primarily by the fusion of hydrogen. Fortunately this is quite a stable process so that stars find an equilibrium state (radius) maintained by the balance of radiation pressure and gravitational forces. This stable state has the relation between mass and energy stated above.

B. Phonons

Phonons are lattice vibrations in crystals. The longitudinal vibrations in a crystal can be described by Hooke's law springs connecting all of the atoms in the crystal. The longitudinal vibrations are called acoustic modes as they are the modes that carry sound waves and the direction of vibration is in the same direction as the wave propagation. Transverse modes also exist and they are called optical modes by analogy with light waves that have EM oscillations that are transverse to the direction of wave propagation.

At low frequencies or long wavelengths, the acoustic phonon modes obey the dispersion relation $\epsilon_p = p v_s$, where v_s is the velocity of sound. The low temperature thermodynamics due to lattice vibrations is dominated by the acoustic modes as the optical modes are much higher in energy. The chemical potential of these modes is zero as there is an infinite set of zero energy modes that are available, as in the photon case.

Two simple models for the thermodynamics of lattice vibrations are the Einstein model and the Debye model. The Einstein model treats the vibrations in a lattice of N atoms as N independent d-dimensional harmonic oscillators. The Debye model, which is more accurate, treats the phonons as a set of Bose particles in a box with volume $V = L^d$. Accurate calculations of the true phonon modes in crystals may be carried out computationally, and then the thermodynamics can be calculated numerically. Here we analyse the Debye model.

Consider a Debye model for a cubic lattice with N atoms. The volume is $V = L^3$. As remarked above, analysis of the acoustic phonons uses the dispersion relation $\epsilon_p = v_s p$ and chemical potential $\mu = 0$, so $z = 1$. So far this model looks exactly the same as the photon model described above, however there is an important difference, the number of acoustic phonon modes in the model is set to $3N$ to ensure a correct crossover to the high temperature limit. This is correct at high temperature as there the optical and acoustic phonons contribute. To enforce a limit on the possible number of phonons, we add a constraint to the calculations,

$$N = (\frac{L}{2\pi})^3 \frac{4\pi k_D^3}{3} \qquad \text{or} \qquad k_D = \left(\frac{6\pi^2 N}{V}\right)^{1/3} \tag{138}$$

which is mathematically similar to the definition of the Fermi wavevector, however the physics here is quite different. The expressions for the thermodynamics looks similar to those for photons in a box, with the modification that the upper limit of the integrations over p is now $p_D = \hbar k_D$, so we have,

$$ln(\Xi) = -3 \left(\frac{L}{2\pi\hbar}\right)^3 \int_0^{p_D} 4\pi p^2 dp \; ln(1 - e^{-\beta p v_s}), \tag{139}$$

where the factor of three in front of this expression is to capture the correct number of degrees of freedom in the high temperature limit. At enough temperatures the optic phonons may freeze out leading to only N active phonon modes.

The internal energy is given by,

$$U = 3 \left(\frac{L}{2\pi\hbar}\right)^3 \int_0^{p_D} 4\pi p^2 dp \; (p v_s) \frac{e^{-\beta p v_s}}{1 - e^{-\beta p v_s}} = V \int d\omega \; u(\omega) \tag{140}$$

where $n(\omega)$ is the number density of phonons and $u(\omega)$ is the energy density at angular frequency ω. Notice that the additional terms, $ln(1 - z)$ and $z/(1 - z)$ are again omitted, as an infinite number of acoustic phonons with zero energy makes no contribution to the physics of the problem. We define the Debye temperature,

$$k_B T_D = p_D v_s; \qquad \text{so that} \qquad T_D = \frac{h v_s}{2 k_B} \left(\frac{6N}{\pi V}\right)^{1/3} \tag{141}$$

so that,

$$\frac{U}{N k_B} = 9T \left(\frac{T}{T_D}\right)^3 \int_0^{T_D/T} dx \frac{x^3}{e^x - 1} \tag{142}$$

The specific heat is the most directly measurable thermodynamic quantity for phonons, so we consider its behavior in the low and high temperature limits. At low temperatures, the upper limit of the integral goes to infinity and the integral is carried out using Eq. (132). In the high temperature limit T_D/T is small, so we take the leading order term in x of Eq. (144), so we replace the denominator by x. The limiting behaviors of the specific heat within the Debye model are then,

$$\frac{C_V}{N k_B} \to \frac{12\pi^4}{5} \left(\frac{T}{T_D}\right)^3 \qquad \text{for} \qquad T << T_D \tag{143}$$

and

$$\frac{C_V}{Nk_B} \to \frac{\partial}{\partial T}\left(9T\left(\frac{T}{T_D}\right)^3 \int_0^{T_D/T} dx\, \frac{x^3}{x}\right) = 3 \quad T \gg T_D. \tag{144}$$

The high temperature result may be understood as the equipartition theorem applied to both the spatial and momentum degrees of freedom, when both are harmonic. There are then six modes (3 momentum and 3 position) with internal energy $k_B T/2$ for each mode.

To demonstrate this explicity, consider the general problem of N particles with N different masses m_i, and N phonon models with N different spring constants k_i, so the Hamiltonian is,

$$H = \sum_i \frac{p_i^2}{2m_i} + \sum_i \frac{1}{2}k_i x_i^2 \tag{145}$$

The classical cannonical partition function for this system is,

$$Z = \prod_{i=1}^N \int_{-\infty}^{\infty} d^d x_i e^{-\beta k_i \vec{x}_i^2/2} \prod_{i=1}^N \int_{-\infty}^{\infty} d^d p_i e^{-\beta \vec{p}_i^2/2m_i} \tag{146}$$

where d is the spatial dimension. Integration yields,

$$Z = \frac{\prod_{i=1}^N (\alpha_i)^d}{N! \prod_{i=1}^N (\lambda_i)^d}; \qquad \text{where} \quad \lambda_i = \frac{h^2 \beta}{2\pi m_i}; \quad \alpha_i = \frac{2\pi}{\beta k_i} \tag{147}$$

It is convenient to define $a_i = \alpha_i * \sqrt{\beta}$ and $b_i = \lambda_i/\sqrt{\beta}$ to be independent of β, so that,

$$F = -\frac{1}{\beta}ln(Z) = -\frac{1}{\beta}\left[ln\left(\frac{\prod_{i=1}^N (a_i)^d}{N! \prod_{i=1}^N (b_i)^d}\right) - dNln(\beta)\right] = -\frac{1}{\beta}[C - dNln(\beta)] \tag{148}$$

and

$$U = -\frac{\partial}{\partial \beta}(ln(Z)) = -\frac{\partial}{\partial \beta}(-dNln(\beta)) = dNk_B T \tag{149}$$

This is a general proof of the equipartition theorem for harmonic systems and it shows that no matter what the mass of the particles or stiffness of the springs, the energy per harmonic mode is $k_B T/2$. This is true for classical harmonic momenta and for classical harmonic potentials. Note also that the quantum mechanical treatment of phonons lead to dispersion relation that looks like the relativistic dispersion relation, though the potential in which the vibrations are occuring in a classical harmonic potential, and their velocities are non-relativistic so we are justified in using the classical non-relativistic calculation for the high temperature limit.

The Debye temperature is an important parameter in materials as it is a rough measure of the elastic properties and melting temperature of the material. A high Debye temperature indicates a stiff material with a high melting temperature (e.g. for diamond $T_D \approx 2200K$, while a low Debye temperature indicates a soft material with a low melting temperature (e.g. for lead $T_D = 105K$. Calorimetry measurements of C_V are quite routine and if they are carried out over a temperature range $0 < T < 5T_D$, they clearly show the crossover between the two regimes of Eqs. (143) and (144).

III. MODELING OF THE BEHAVIOR OF METALS

In some metals the electrons near the Fermi energy can be treated as a free Fermi gas. For example, this approximation is very good Alkali metals that have one electron in an outer s orbital. The free electron model is also a good starting point for more complex metals where band structure effects become important and for strongly correlated systems where Coulomb interactions between the electrons plays a key role. In many materials the Debye model provides a useful approximation of the contribution of phonons to the thermodynamic properties. The thermodynamic behavior of metals can therefore, to first approximation, be considered to be a sum of the contribution due to phonons and a contribution due to electrons. For the specific heat this leads to the prediction that at low temperatures,

$$\frac{C_V}{Nk_B} = \frac{\pi^2}{2}\frac{k_B T}{\epsilon_F} + \frac{12\pi^4}{5}\left(\frac{T}{T_D}\right)^3 \tag{150}$$

which is a sum of the electron contribution from Eq. (91) and the phonon contribution from Eq. (143). This provides a good approximation when band structure effects, interaction effects and disorder effects are not important, and provided $T << T_D$ and $kT << E_F$. Note that the Fermi wavevector is changed to $k_F = (3\pi^2 N/V)^{1/3}$ to take account of the fact that electrons can have either up or down spin, whereas the derivation leading up to Eq. (91) did not take the spin of the electron into account.

The magnetic behavior of the free electron gas also provides a good first approximation to many interesting solid state systems. Below we consider the behavior in two cases: first the limit of low field where we calculate the zero field magnetic susceptibility in the low and high temperature limits and; second the high field limit where fascinating oscillatory behavior can occur due to the occurance of pronounced Landau levels. Oscillations due to Landau levels are used to map out the Fermi surface of metals (the de Haas van Alphen effect), and they lead to particularly strong effects in to two dimensions where new states of matter arise in the integer and fractional quantum Hall effects.

A. Magnetic susceptibility in the low field limit

There are two contributions to the magnetic response of the free electron gas in the presense of an applied magnetic field B. Since the electrons have spin, there is a "Zeeman" splitting of the system into up electrons and down electrons that have different response to the magnetic field. This response is called Pauli paramagnetism. We will calculate its contribution below. A second magnetic response occurs even in systems without any magnetic moment due to spin. This response occurs due to the fact that when a charge moves it induces a magnetic field. For example, since the electron is charged when it moves in a circular orbit, it produces an "orbital" magnetic moment, μ_o, that is equal to

$$\vec{\mu}_o = IA\hat{n} = -\frac{e}{2m_e}\vec{L} \tag{151}$$

where I is the orbital current, A is the area of the circuit and $\vec{L}$ is the angular momentum. When a magnetic field is applied to the system, Lenz's law tells us that the system tries to avoid the change in the magnetic field, so the response is to oppose the applied field. This is particularly strong in superconductors where supercurrents respond to completely screen out the applied magnetic field in the the low field regime. In normal metals the response is much weaker, but nevertheless the system responds by setting up currents to oppose an applied field. The general effect of setting up currents to oppose a magnetic field when it is applied to a material is called "Landau" diamagnetism. We now calculate the Pauli paramagnetic and Landau diamagnetic contributions to the magnetism of the free electron gas at low temperatures. These contributions are treated separately and the overall response is a sum of the two, to first approximation.

1. Pauli paramagnetism, magnetic susceptibility at low field

At high temperatures, a classical gas of particles that have spin has the magnetic susceptibility of an Ising paramagnet, so Eq. (97) applies $\chi(T \to \infty) = \mu_s^2/k_B T$. Note that in Eq. (97) and below χ is the magnetic susceptibility per spin. The high temperature behavior of the electron system is the same. However, as usual, the low temperature behavior is very different. The Pauli paramagnet model considers only the spin of the electron, so the energy levels are given by,

$$\epsilon_{p,S} = \frac{\vec{p}^2}{2m} - \vec{\mu}_s \cdot \vec{B}S \tag{152}$$

where $S = \pm 1$ and μ_s is one half the magnetic moment of the electron. The Fermi energy is fixed by the conditions,

$$\epsilon_F = \frac{\hbar^2 k_+^2}{2m} + \mu_s B = \frac{\hbar^2 k_-^2}{2m} - \mu_s B \tag{153}$$

and,

$$N_+ = \left(\frac{L}{2\pi}\right)^3 \frac{4\pi}{3} k_+^3; \quad \text{and} \quad N_- = \left(\frac{L}{2\pi}\right)^3 \frac{4\pi}{3} k_-^3 \tag{154}$$

we also define,

$$k_F = (3\pi^2 \frac{N}{V})^{1/3}; \quad \epsilon_F = \frac{\hbar^2 k_F^2}{2m} \tag{155}$$

which are the Fermi momentum and Fermi energy in zero field. We then have,

$$N_+ = \frac{4\pi V}{3h^3}[2m(\epsilon_F + \mu_s B)]^{3/2}; \qquad N_- = \frac{4\pi V}{3h^3}[2m(\epsilon_F - \mu_s B)]^{3/2} \tag{156}$$

The magnetization is

$$M = \mu_s(N_+ - N_-) = \mu_s \frac{4\pi V}{3h^3}(2m)^{3/2}[(\epsilon_F + \mu_s B)^{3/2} - (\epsilon_F - \mu_s B)^{3/2}] \tag{157}$$

so the zero field susceptibility is,

$$\chi(T \to 0) = \frac{1}{N}\frac{\partial M}{\partial B}|_{B\to 0} = \frac{V}{N}\frac{4\pi\mu_s^2(2m)^{3/2}\epsilon_F^{1/2}}{h^3} = \frac{3}{2}\frac{\mu_s^2}{\epsilon_F} \tag{158}$$

B. Landau diamagnetism, Landau levels, de Haas van Alphen and QHE

The energy spectrum of a non-interacting Fermi gas in a magnetic field is given by,

$$\epsilon_{p_z,j} = \frac{e\hbar B}{m}(j + \frac{1}{2}) + \frac{p_z^2}{2m} = \hbar\omega_c(j + \frac{1}{2}) + \frac{p_z^2}{2m} \tag{159}$$

where $\omega_c = eB/m$ is the Cyclotron frequency. In doing this calculation, we assumed that the magnetic field is along the z direction. The electrons in a magnetic field make circular orbits in the x-y plane and the result above is found by solving the Schrodinger equation with the replacement $\vec{p} \to \vec{p} - e\vec{A}$, where $\vec{A}$ is the vector potential. The cyclotron frequency can be found by considering classical circular motion,

$$qvB = mv^2/r; \qquad \text{so that} \qquad \omega = qB/m \tag{160}$$

In our case the charge is e. The direction of the orbital motion is to oppose the applied field.

Each of the harmonic oscillator energy levels is called a Landau level and has degeneracy,

$$g = \phi/\phi_0 = BL_xL_y/(h/e) \tag{161}$$

(see Huang 253-271). The degeneracy is related to flux quantization, which states that in a phase coherent free electron quantum system, the smallest unit of flux is the flux quantum h/e (note that in superconductors it is $h/2e$ due to fact that the elementary charge carrier is a Cooper pair with charge $q = -2e$). This has the same physical origin as the Aharonov-Bohm effect which states that even in regions of space where there is no magnetic field, the magnetic potential has an effect on the phase of the wavefunction. Therefore if we make a loop in a region of space that contains no magnetic field, but which encloses some magnetic field we find,

$$\delta\theta = \frac{q}{\hbar}\oint \vec{A} \cdot d\vec{l} = \frac{q}{\hbar}\phi \tag{162}$$

where $\phi = \int \vec{B} \cdot d\vec{a}$. The phase appears in wavefunction as $e^{i\theta}$ and the wavefunction should be the same if we make a loop, so $\delta\theta(loop) = 2\pi n$, with n an integer. This implies that the enclosed flux must have the form,

$$\phi = \frac{h}{e}n = \phi_0 n \tag{163}$$

where $\phi_0 = h/e$ is the flux quantum for electrons.

Landau showed that spinless Fermions can exhibit magnetic response through the response of their orbitals to an applied magnetic field. This is demonstrated by calculating the magnetic susceptibility using the energy levels above. The grand partition function for this system is,

$$\Xi = \prod_{p_z,j} \sum_{n_{p_z,j}} (e^{-\beta(\epsilon_{p_z,j}-\mu)n_{p_z,j}})^g \tag{164}$$

so that,

$$ln(\Xi) = \frac{2gL_z}{h}\int_{-\infty}^{\infty}\sum_{j=0}^{\infty} ln\left(1 + zExp[-\beta(\hbar\omega_c(j + \frac{1}{2}) + \frac{p_z^2}{2m})]\right) \tag{165}$$

At high temperatures, z is small and to leading order in z, we find,

$$ln(\Xi) = \frac{2gL_z}{h} \int_{-\infty}^{\infty} \sum_{j=0}^{\infty} z Exp[-\beta(\hbar\omega_c(j+\frac{1}{2}) + \frac{p_z^2}{2m})] = \frac{2gL_z}{h} \left(\frac{2\pi m}{\beta}\right)^{1/2} z \sum_{j=0}^{\infty} Exp[-\beta\hbar\omega_c(j+\frac{1}{2})] \tag{166}$$

The sum is a geometric progression, so it may be summed to find,

$$ln(\Xi) = \frac{gL_z}{h} \left(\frac{2\pi m}{\beta}\right)^{1/2} z \frac{1}{sinh(x)} = \frac{BAL_z}{(h/e)} \frac{1}{\lambda^3} \frac{h^2}{2\pi m k_B T} z \frac{1}{sinh(x)} = \frac{Vz}{\lambda^3} \frac{x}{sinh(x)} \tag{167}$$

where $x = \beta\hbar\omega_c/2 = \beta\mu_0 B$. We then have,

$$N = z\frac{\partial}{\partial z}ln(\Xi) = \frac{zV}{\lambda^3}\frac{x}{sinh(x)}; \qquad \text{where} \qquad x = \beta\mu_o B \tag{168}$$

and μ_o is the effective magnetic moment and has a form similar to the Bohr magneton. The magnetization is given by,

$$M = \frac{1}{\beta}\frac{\partial}{\partial B}(ln(\Xi)) = \frac{zV}{\lambda^3}\mu_o\left[\frac{1}{sinh(x)} - \frac{x cosh x}{sinh^2(x)}\right] = -N\mu_o L(x) \tag{169}$$

where $L(x) = coth(x) - 1/x$ is the Langevin function.

If the field energy is small compared to the thermal energy, $\mu B << k_B T$, then we find,

$$z \approx \frac{\lambda^3 N}{V}; \qquad M \approx -\frac{N\mu_o B}{3k_B T}; \qquad \chi(T \to \infty) = \frac{1}{N}\frac{\partial M}{\partial B} = -\frac{\mu_o^2}{3k_B T} \tag{170}$$

The total susceptibility at high temperatures is then as sum of the paramagnetic and diamagnetic contributions,

$$\chi(T \to \infty, h \to 0) = \frac{1}{k_B T}[\mu_B^2 - \frac{1}{3}\mu_o^2] \tag{171}$$

It can be shown (see Pathria and Beale Eq. (48)) that at low temperatures and small fields, the diamagnetic contribution at zero temperature is,

$$\chi(T \to 0) = -\frac{1}{2\epsilon_F}\mu_o^2 \tag{172}$$

so that at zero temperature the sum of the paramagnetic and diamagnetic contributions to the magnetic susceptibility per spin is,

$$\chi(T \to 0, h \to 0) = \frac{1}{\epsilon_F}[\frac{3}{2}\mu_B^2 - \frac{1}{2}\mu_o^2] \tag{173}$$

C.   Strong fields

In strong fields, the Landau levels are highly degenerate because ϕ/ϕ_0 is large. In this limit novel effects occur as the magnetic field sweeps through conditions where a Landau level is filled and a new Landau level begins being filled. The most dramatic effects occur in two-dimensional systems, but very important effects also occur in bulk samples. Due to this effect, bulk single crystal metal samples in strong fields (typically several Tesla) and at low temperatures ($\mu B > k_B T$) exhibit oscillations of most physical properties as the magnetic field is varied. Oscillations in the magnetic moment are called the de Haas - van Alphen effect, oscillations in resistivity Shubnikov-de Haas oscillation. Oscillations also occur in the specific heat and other physical properties. In crystals dHvA oscillations can be used to map the Fermi surface of the metal and also to determine the carrier density.

However the most pronounced effects occur in two dimensions where the integer and fractional quantum Hall effects are observed. A starting point for understanding the two dimensional case in strong fields is as follows. Consider a system with N electrons. In two dimensions the energy levels are $\hbar\omega_c(n + 1/2)$. We define n_F to be the number of Landau levels that must be filled or partially filled to accomodate N electrons in the system,

$$n_F = \frac{N}{2g}; \quad \text{and} \quad \epsilon_F = \hbar\omega_c(n_F + \frac{1}{2}) \tag{174}$$

Interesting physics occurs when we change the magnetic field because n_F changes from n to $n-1$ at a special field B_n given by,

$$\frac{N}{2g} = n - 1 = \frac{N(h/e)}{2AB_n}; \quad \text{so} \quad B_n = \frac{1}{2(n-1)}\frac{N}{A}\frac{h}{e} \tag{175}$$

In doing this calculation we have not taken into account Zeeman splitting. To take this into account, each of the Landau levels is further split into two levels, with energies

$$\hbar\omega_c(n + \frac{1}{2}) - \mu_s B; \quad \text{and} \quad \hbar\omega_c(n + \frac{1}{2}) + \mu_s B. \tag{176}$$

Zeeman splitting is important at high fields and in the low n regime.

Assigned problems and sample quiz problems

Sample Quiz Problems

Quiz Problem 1. Write down the equation for the thermal de Broglie wavelength. Explain its importance in the study of classical and quantum gases.

Quiz Problem 2. Why are the factors $1/N!$ and $1/h^{3N}$ introduced into the derivation of the partition function of the ideal classical gas?

Quiz Problem 3. By using the fact the $g_{3/2}(1) = \zeta(3/2) = 2.612$ and using,

$$N = \frac{V}{\lambda^3}g_{3/2}(z) + \frac{z}{1-z} = N_1 + N_0 \tag{177}$$

find an expression for the critical temperature of the ideal Bose gas.

Quiz Problem 4. State and give a physically explanation of the behavior of the chemical potential μ and the fugacity $z = e^{\beta\mu}$ as temperature $T \to \infty$, for both the Bose and Fermi gases.

Quiz Problem 5. State and give a physical explanation of the behavior of the chemical potential μ and the fugacity $z = e^{\beta\mu}$ as temperature $T \to 0$, for both the Bose and Fermi gases.

Quiz Problem 6. Write down the starting expression in the derivation of the grand partition function, Ξ_F for the ideal Fermi gas, for a general set of energy levels ϵ_l. Carry out the sums over the energy level occupancies, n_l and hence write down an expression for $ln(\Xi_F)$.

Quiz Problem 7. Write down the starting expression in the derivation of the grand partition function, Ξ_B for the ideal Bose gas, for a general set of energy levels ϵ_l. Carry out the sums over the energy level occupancies, n_l and hence write down an expression for $ln(\Xi_B)$.

Quiz Problem 8. (i) Find the single particle energy levels of a non-relativistic quantum particle in a box in 3-d. (ii) Given that

$$ln(\Xi_B) = -\sum_l ln(1 - ze^{-\beta\epsilon_l}), \tag{178}$$

using the energies of a quantum particle in a box found in (i), take the continuum limit of the energy sum above to find the inegral form for $ln(\Xi_B)$. Don't forget the ground state term.

Quiz Problem 9. White dwarf stars are stable due to electron degeneracy pressure. Explain the physical origin of this pressure.

Quiz Problem 10. In the condensed phase superfluids are often discussed in terms of a two fluid model. Based on the analysis of the ideal Bose gas, explain the physical basis of the two fluid model.

Quiz Problem 11. Why is the chemical potential of photons in a box, and also acoustic phonons in a crystal, taken to be zero?

Quiz Problem 12. Write down the blackbody energy density spectrum.

Quiz Problem 13. Write down and explain the relationship between the intensity of radiation emitted by a blackbody (Stefan-Boltzmann law) and the energy density of a photon gas in the blackbody.

Quiz Problem 14. Explain the physical origin of the cosmic microwave background (CMB) blackbody spectrum of the universe. It is currently at a temperature of $T_{CMB} = 2.713K$. If the universe is expanding at a constant rate $L(t) = H_0 t$, where H_0 is a constant what is the expected behavior of the temperature $T_{CMB}(t)$.

Quiz Problem 15. Explain the physical origins of the paramagnetic and diamagnetic behaviors of the free electron gas.

Quiz Problem 16. Derive or write down the spectral energy density for blackbody radiation in a universe with two spatial dimensions.

Quiz Problem 17. Derive or write down the Debye theory for the internal energy for phonons in a square lattice. Derive the low and high temperature limits of the internal energy and specific heat for this system.

Quiz Problem 18. Find the leading order term in the temperature dependence of the internal energy and specific heat of an ultrarelativistic Fermi gas at low temperature.

Assigned problems

Assigned Problem 1. From the density of states for an ideal monatomic gas $\Omega(E)$ given in Eq. (22) of the notes, find the Sackur-Tetrode equation for the entropy, Eq. (23) of the notes.

Assigned Problem 2. Using the canonical partition function for the ideal gas, show that,

$$(\delta E)^2 = k_B T^2 C_v \tag{179}$$

Assigned Problem 3. Using the grand partition function of the ideal classical gas show that,

$$(\delta N)^2 = N k_B T \rho \kappa_T \tag{180}$$

Assigned Problem 4. At high temperatures we found that the ideal quantum gases reduce to the ideal classical gases. Derive the next term in the expansion of the equation of state of the ideal Fermi gas at high temperatures, and verify that,

$$\frac{PV}{Nk_BT} = 1 + \frac{1}{2^{5/2}}\frac{\lambda^3 N}{V} + ... \tag{181}$$

The pressure of the ideal Fermi gas is higher than that of the classical gas at the same temperature and volume. Why? Carry out a similar expansion for the Bose gas. Is the pressure higher or lower than the ideal classical gas at the same values of T, V? Why?

Assigned Problem 5. By expanding the denominator of the integral, $1/(1-y)$ for small $y = ze^{-x^2}$ show that,

$$f_{3/2}(z) = \frac{4}{\pi^{1/2}}\int_0^\infty dx\ x^2 \frac{ze^{-x^2}}{1+ze^{-x^2}} = \sum_{l=1}^\infty \frac{(-1)^{l+1}z^l}{l^{3/2}} \tag{182}$$

Assigned Problem 6. Derive expressions for Z, Ξ, PV, μ and U for the classical gas in one and two dimensions. Are the results what you expect? How do they compare with the result in three dimensions. White general expressions

that are valid in any dimension.

Assigned Problem 7. Derive expressions for Ξ, PV, N/V and U for the Bose gas in one and two dimensions. White general expressions that are valid in any dimension. Find the leading order terms in the high temperature expansions for these quantities. Are the results what you expect? How do they compare with the result in three dimensions and with the classical behavior.

Assigned Problem 8. Derive expressions for Ξ, PV, N/V and U for the Fermi gas in one and two dimensions. White general expressions that are valid in any dimension. Find the leading order terms in the high temperature expansions for these quantities. Are the results what you expect? How do they compare with the result in three dimensions, and with the classical gas.

Assigned Problem 9. Using the results of Problem 7, discuss the behavior of the Bose gas at low temperatures in one and two dimensions. Is a finite temperature Bose condensation predicted ? Explain your reasoning.

Assigned Problem 10. Using the results of Problem 8, discuss the behavior of the Fermi gas at low temperatures in one and two dimensions. Is there different behavior as a function of dimension? Explain your reasoning.

Assigned Problem 11. For the 3-D non-relativistic case: a) Find the entropy of the ideal Bose gas in the condensed phase $T < T_c$. b) Find the entropy of the ideal Fermi gas at low temperatures to leading order in the temperature. Does the Fermi or Bose gas have higher entropy at low temperatures? Why?

Assigned Problem 12. Show that a $d - dimensional$ Bose gas with dispersion relation $\epsilon_p = cp^s$ obeys the relation,

$$P = \frac{s}{d}\frac{U}{V} \tag{183}$$

Assigned Problem 13. By expanding Eq. (II.103) of the lecture notes to fourth order in y, show that it reproduces $-f_R(y)$ as given in Eq. (II.111).

Assigned Problem 14. Write down the 4×4 transfer matrix for two ising chains connected together. Show that this transfer matrix can be written in the form,

$$\hat{T} = (\hat{M}_2)(\hat{M}_1 \otimes \hat{M}_1) \tag{184}$$

where $\hat{M}_1$ is the transfer matrix of the Ising chain, while $\hat{M}_2$ is a 4×4 diagonal matrix. $\otimes$ is the direct or Kronecker product.

Assigned Problem 15. Use the transfer matrix method to find the partition function for the one dimensional Ising model in a magnetic field h. From your expression find the magnetic susceptibility at $h = 0$. Does it obey a Curie Law?

Assigned Problem 16. Find the thermodynamic properaties, PV, U, S, C_V, N of a photon gas in d dimensions. Show that the entropy per photon is independent of temperature.

Assigned Problem 17. Find the thermodynamic properties, PV, U, S, C_V of the Debye phonon model in d dimensions.

Assigned Problem 18. Consider a two dimensional electron gas in a magnetic field that is strong enough so that all of the particles can be accomodated in the lowest Landau level. Taking into account both the paramagnetic and diamagnetic contributions, find the magnetization at temperature $T = 0K$.

Assinged Problem 19. (Optional) Show that the low temperature specific heat of the relativistic Fermi gas in three dimensions is given by,

$$\frac{C_V}{Nk_B} = \frac{\pi^2(x^2 + 1)^{1/2}}{x^2}\frac{k_BT}{m_0c^2}; \quad \text{where} \quad x = p_F/(m_0c) \tag{185}$$