Homework 5: Phys 7230 (Spring 2022)

Tien Vo

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***Problem* 1** (Quantum many-body statistics)**:** Consider a system with 3 single particle nondegenerate energy levels $\alpha = (a, b, c)$ equally spaced with values $\epsilon_a = 0, \epsilon_b = \epsilon, \epsilon_c = 2\epsilon$, and occupied by 2 particles.

(a) Write down the *ground* states for bosons and fermions in three forms:

(i) Many-body wavefunction $\psi_{\alpha_1,\alpha_2}(x_1, x_2)$, in terms of *normalized* single particle wavefunctions $\psi_\alpha(x)(\alpha = (a, b, c))$, appropriately (anti-)symmetrized using determinant and permanent method. Make sure that there is a correct overall normalization.

(ii) A many-body ket in the occupation basis $\{n_\alpha\}$ representation, written as, $|n_a, n_b, n_c\rangle = |n_a\rangle |n_b\rangle |n_c\rangle$.

(iii) Drawing equally spaced energy levels $\epsilon_a, \epsilon_b, \epsilon_c$ as horizontal lines with "balls" representing particles sitting on the levels.

Solution.

(i) For fermions, the ground state has energy ϵ since they cannot both occupy a. Thus, the wave function is

$$\psi^F_{a,b}(x_1, x_2) = \frac{1}{\sqrt{2}} \det \begin{bmatrix} \psi_a(x_1) & \psi_a(x_2) \\ \psi_b(x_1) & \psi_b(x_2) \end{bmatrix} = \frac{1}{\sqrt{2}} \big(\psi_a(x_1)\psi_b(x_2) - \psi_a(x_2)\psi_b(x_1)\big). \tag{1.1}$$

For bosons, they can both occupy a. Thus, the ground state wave function is

$$\psi^B_{a,a}(x_1, x_2) = \frac{1}{2} \mathrm{Perm} \begin{bmatrix} \psi_a(x_1) & \psi_a(x_2) \\ \psi_a(x_1) & \psi_a(x_2) \end{bmatrix} = \psi_a(x_1)\psi_a(x_2). \tag{1.2}$$

(ii) $\left|\psi^F_{a,b}\right\rangle = |1, 1, 0\rangle$ and $\left|\psi^B_{a,a}\right\rangle = |2, 0, 0\rangle$. □

(b) Repeat above many-body state description for the 1st *excited* many-body states for bosons and fermions.

Solution.

(i) The first excited state for fermions has total energy 2ϵ

$$\psi^F_{a,c}(x_1, x_2) = \frac{1}{\sqrt{2}} \big(\psi_a(x_1)\psi_c(x_2) - \psi_a(x_2)\psi_c(x_1)\big), \tag{1.3}$$

where we have simply exchanged $b \to c$ from the previous result. For bosons, one particle occupies a and the other is excited to b,

$$\psi^B_{a,b}(x_1, x_2) = \frac{1}{\sqrt{2}} \mathrm{Perm} \begin{bmatrix} \psi_a(x_1) & \psi_a(x_2) \\ \psi_b(x_1) & \psi_b(x_2) \end{bmatrix} = \frac{1}{\sqrt{2}} \big(\psi_a(x_1)\psi_b(x_2) + \psi_a(x_2)\psi_b(x_1) \big). \tag{1.4}$$

(ii) $\left| \psi^F_{a,c} \right\rangle = |1, 0, 1\rangle$ and $\left| \psi^B_{a,b} \right\rangle = |1, 1, 0\rangle$. □

(c) Using $|n_a, n_b, n_c\rangle$ labeling list (i) *all* the many-body eigenstates for this system of 2 particles for bosons and for fermions, (ii) corresponding many-body energies $E_{\{n_\alpha\}} = E_{n_a,n_b,n_c}$, and (iii) the 2-particle partition function Z, explicitly writing out the sum of all finite number of terms. Do this for both bosons and fermions.

Solution.
(i)

- Fermions: $|1, 1, 0\rangle, |1, 0, 1\rangle, |0, 1, 1\rangle$
- Bosons: $|2, 0, 0\rangle, |1, 1, 0\rangle, |0, 2, 0\rangle, |1, 0, 1\rangle, |0, 1, 1\rangle, |0, 0, 2\rangle$

(ii)

- Fermions: $E_{1,1,0} = \epsilon$, $E_{1,0,1} = 2\epsilon$, $E_{0,1,1} = 3\epsilon$
- Bosons: $E_{2,0,0} = 0$, $E_{1,1,0} = \epsilon$, $E_{0,2,0} = E_{1,0,1} = 2\epsilon$, $E_{0,1,1} = 3\epsilon$, $E_{0,0,2} = 4\epsilon$

(iii) For fermions, there is no degeneracy, so

$$Z^F = \sum_{\{q\}} e^{-\beta E_q} = e^{-\beta\epsilon} + e^{-2\beta\epsilon} + e^{-3\beta\epsilon}. \tag{1.5}$$

For bosons,

$$Z^B = 1 + e^{-\beta\epsilon} + 2e^{-2\beta\epsilon} + e^{-3\beta\epsilon} + e^{-4\beta\epsilon}. \tag{1.6}$$

□

(d) Using quantum many-body state labeling $|\alpha_1, \alpha_2\rangle$ where α_i is the single-particle state (a, b, or c) occupied by *distinguishable* particle $i = (1, 2)$, write down (i) *all* many-body states for *distinguishable* particles, (ii) their corresponding many-body energies E_{α_1,α_2}, and (iii) the 2-particle partition function $Z_{N=2}$. Show that this latter sum in Z_2 of many terms can actually be written as a product of 1-particle partition functions, i.e., $Z_2 = Z_1^2$.

Solution.
(i) $|a, a\rangle, |b, b\rangle, |c, c\rangle, |a, b\rangle, |b, a\rangle, |a, c\rangle, |c, a\rangle, |b, c\rangle, |c, b\rangle$. (ii) $E_{a,a} = 0, E_{a,b} = E_{b,a} = \epsilon, E_{a,c} = E_{c,a} = E_{b,b} = 2\epsilon, E_{b,c} = E_{c,b} = 3\epsilon, E_{c,c} = 4\epsilon$. (iii) It follows from (i) and (ii) that

$$Z_2 = 1 + 2e^{-\beta\epsilon} + 3e^{-2\beta\epsilon} + 2e^{-3\beta\epsilon} + e^{-4\beta\epsilon}. \tag{1.7}$$

For a single particle, the partition function is

$$Z_1 = 1 + e^{-\beta\epsilon} + e^{-2\beta\epsilon}. \tag{1.8}$$

Thus, we also have

$$\begin{aligned} Z_1^2 &= 1 + 2e^{-\beta\epsilon} + 2e^{-2\beta\epsilon} + \left(e^{-\beta\epsilon} + e^{-2\beta\epsilon}\right)^2 \\ &= 1 + 2e^{-\beta\epsilon} + 2e^{-2\beta\epsilon} + e^{-2\beta\epsilon} + e^{-4\beta\epsilon} + 2e^{-3\beta\epsilon} \\ &= 1 + 2e^{-\beta\epsilon} + 3e^{-2\beta\epsilon} + 2e^{-3\beta\epsilon} + e^{-4\beta\epsilon} \\ &= Z_2. \end{aligned} \tag{1.9}$$

$\square$

***Problem* 2** (Bose gas in a box)**:** In lectures we introduced noninteracting (ideal) Bose gas in a box (with periodic boundary conditions) and presented many results, some without derivations. Here I will ask you to derive some of the details.

(a) Following our derivation of the number equation $\overline{N}$, Eq. 24 from its definition Eq. 22 in the lecture notes, from the grand canonical partition function derive the equation of state for the pressure P, Eq. 29 and energy E, Eq. 30, Combining these results together with $\overline{N}$, Eq. 24, in 3D, derive the first two virial coefficients for the equation of state (Eq. 31) at high temperature $T \gg T_*$ (nondegenerate gas limit), where $z \ll 1$. Show that $a_0 = 1$ and $a_1 = -1/2^{5/2}$, as found in Eq. 18 of the notes.

Hint: This can be done by a powerful and quite general iterative perturbation series approach, valid when $z \ll 1$. Suppose you want to solve the number equation, $n = g(z) = c_1 z + c_2 z^2 + \ldots$, inverting it for $z(n)$ (so you can later eliminate z from other thermodynamics quantities like P). Take the zeroth order approximation $z \approx z_1$ ignoring z^2 and higher order terms, then the equation above gives $z_1 = n/c_1$. Then at next iteraction of the approximation, you can find z_2 by going to 2nd order in z expansion of $g(z)$, using the unknown z_2 inside $c_1 z$ but only using the previous 1st order solution z_1 inside $c_2 z^2$ and solving for z_2, etc. Why do you think this is justified? This way you will find, $z \approx z_2 = b_1 n + b_2 n^2$, which is sufficient to compute $P(T, n)$ to 2nd order in n by eliminating z in its Taylor expansion in right hand side of Eq. 31.

Solution.

First, we calculate the free energy (27) in the notes.

$$
\begin{aligned}
\mathcal{F}_B &= k_B T \sum_{\mathbf{k}} \ln\left[1 - e^{-(\epsilon_{\mathbf{k}}-\mu)/k_B T}\right] \\
&= k_B T \left(\frac{L}{2\pi}\right)^d \int d^d k \ln\left[1 - e^{-(\epsilon-\mu)/k_B T}\right] \\
&= k_B T \left(\frac{L}{2\pi}\right)^d S_d \int_0^\infty dk k^{d-1} \ln\left[1 - e^{-(\epsilon-\mu)/k_B T}\right] \\
&= \frac{V k_B T}{2(2\pi)^d} \left(\frac{2m}{\hbar^2}\right)^{d/2} S_d \int_0^\infty d\epsilon \epsilon^{d/2-1} \ln\left[1 - e^{-(\epsilon-\mu)/k_B T}\right] \qquad (\epsilon = \hbar^2 k^2/2m) \\
&= -\frac{V}{d(2\pi)^d} \left(\frac{2m}{\hbar^2}\right)^{d/2} S_d \int_0^\infty d\epsilon \frac{\epsilon^{d/2}}{e^{(\epsilon-\mu)/k_B T} - 1} \\
&= -\frac{2}{d} \frac{V k_B T}{\Gamma(d/2)} \left(\frac{m k_B T}{2\pi\hbar^2}\right)^{d/2} \int_0^\infty dx \frac{x^{d/2}}{e^x z^{-1} - 1} \\
&= -\frac{2}{d} \frac{V k_B T}{\lambda^d} \frac{\Gamma(d/2+1)}{\Gamma(d/2)} g_{d/2+1}(z) \\
&= -\frac{V k_B T}{\lambda^d} g_{d/2+1}(z). \qquad (2.1)
\end{aligned}
$$

Thus, it follows that

$$
P = -\frac{\mathcal{F}_B}{V} = \frac{k_B T}{\lambda^d} g_{d/2+1}(z). \qquad (2.2)
$$

Similarly, the energy density is

$$\begin{aligned}
\frac{E}{V} &= -\frac{1}{V}\frac{\partial(\ln \mathcal{Z})}{\partial \beta} \\
&= -\frac{1}{V}\sum_{\mathbf{k}} \frac{\partial}{\partial \beta} \ln \left[1 - e^{-(\epsilon-\mu)/k_B T}\right]^{-1} \\
&= \frac{1}{(2\pi)^d}\int d^d k \frac{\epsilon - \mu}{e^{(\epsilon-\mu)/k_B T} - 1} \\
&= \frac{1}{(2\pi)^d}\left(\frac{2m}{\hbar^2}\right)^{d/2}\frac{S_d}{2}\int_0^\infty d\epsilon \frac{\epsilon^{d/2} - \mu\epsilon^{d/2-1}}{e^{(\epsilon-\mu)/k_B T} - 1} \\
&= \frac{k_B T}{\Gamma(d/2)}\left(\frac{m k_B T}{2\pi\hbar^2}\right)^{d/2}\left[\int_0^\infty dx \frac{x^{d/2}}{e^x z^{-1} - 1} - \frac{\mu}{k_B T}\int_0^\infty dx \frac{x^{d/2-1}}{e^x z^{-1} - 1}\right] \\
&= \frac{k_B T}{\lambda^d}\left[\frac{\Gamma(d/2+1)}{\Gamma(d/2)} g_{d/2+1}(z) - g_{d/2}(z)\ln\left(g_{d/2}(z)\right)\right] \\
&\approx \frac{d}{2}\frac{k_B T}{\lambda^d} g_{d/2+1}(z),
\end{aligned} \tag{2.3}$$

where the second term drops out in the limit that $z \ll 1$. Now, from the pressure, in 3D, we can write

$$\frac{PV}{N k_B T} = \frac{g_{5/2}}{g_{3/2}} \approx \frac{z + 2^{-5/2} z^2}{z + 2^{-3/2} z^2} \approx 1 - 2^{-5/2} z. \tag{2.4}$$

But from (25), $n\lambda^3 = g_{3/2} \approx z$, so

$$\frac{PV}{N k_B T} \approx 1 - 2^{-5/2}(n\lambda^3). \tag{2.5}$$

Reading off of this, we know that $a_1 = 1$ and $a_2 = -2^{-5/2}$. □

(b) In lecture I argued that $\mu(T, n)$ is negative for $T \gg T_c$ increases toward zero (with absolute value $|\mu|$ decreasing to 0) with reduced T as it approaches T_c from above. From the defining N equation (23), make the appropriate approximation (assuming $z \ll 1$), neglecting 1 in the denominator of $n^{BE}(\epsilon_{\mathbf{k}})$, do the Gaussian integral over $\mathbf{k}$ and solve for $\mu(T, n)$ in d dimension.

Hint: In Eq. 25, $g_\nu(z) \approx z$ for $z \ll 1$, which is another direct route to your answer above, but use it only as a check.

Solution.

Assuming $\mu \ll 1$, we can write

$$
\begin{aligned}
N &\approx \sum_{\mathbf{k}} e^{-\beta(\epsilon-\mu)} \\
&= z\left(\frac{L}{2\pi}\right)^d \int d^d k \exp\left(-\frac{1}{2}\frac{\beta\hbar^2}{m}k^2\right) \\
&= \frac{zV}{(2\pi)^d}\left[\int dk_j \exp\left(-\frac{1}{2}\frac{\beta\hbar^2}{m}k_j^2\right)\right]^d \\
&= \frac{zV}{(2\pi)^d}\left(\frac{2\pi}{\beta\hbar^2/m}\right)^{d/2} \\
&= zV\left(\frac{mk_BT}{2\pi\hbar^2}\right)^{d/2} \\
&= \frac{zV}{\lambda^d}.
\end{aligned}
\tag{2.6}
$$

Thus, it follows that $z = n\lambda^d$, as expected. Inverting this, we can write

$$
\mu = k_BT \ln\left(n\lambda^d\right). \tag{2.7}
$$

□

(c) Why do I keep saying that at high $T \gg T_c$ the fugacity $z = e^{\mu(T)/T} \ll 1$ in this limit? Use above derived expression for $\mu(T,n)$ to confirm that indeed $z(T \gg T_*) \ll 1$.

Solution.

From above, the fugacity $z \ll 1$ only when $n\lambda^d \ll 1$. This is equivalent to saying $T \gg T_*$. Recall that the degeneracy temperature

$$
k_BT_* = \frac{\hbar^2 n^{2/d}}{2m}, \tag{2.8}
$$

while the temperature defined by the Debye length is

$$
k_BT = \frac{2\pi\hbar^2}{m\lambda^2}. \tag{2.9}
$$

Thus, $k_BT \gg k_BT_*$ only when $n\lambda^d \ll (4\pi)^{d/2} \sim \mathcal{O}(1)$. □

(d) Consider the N, Eq. 23 again. Based on it I argued that as T is lowered and N is increased, μ must increase toward 0, as you verified above. And in addition, in $d > 2$, $\mu(T \to T_c) \to 0$, i.e. gets pinned at $\mu = 0$. Why do I insist on this, namely, why can't μ become positive for $T < T_c$, in its attempt to satisfy the number equation? Argue for this based on Eqs. 22, 33, that for noninteracting Bose gas it is unphysical for μ to become positive.

Hint: Above I asked you to argue that the limiting value of μ is 0. But on the other hand you know that in physics (other than gravity) only *relative* energy matter. Based on your previous argument for $\mu = 0$, for $\epsilon_0 = \hbar^2 k^2/2m$, what do you think the more general answer for the limiting value of μ is in the case of the lowest single-particle energy level $\epsilon_{\alpha=0} = \epsilon_0$ rather than 0?

Solution.

When μ is positive, the integral is still convergent at a finite value. So it is not possible to satisfy the number equation for any arbitrary N. This saturation starts at $\mu = 0$, so the limiting value for μ must be zero. Now, μ is negative for $T \gg T_c$, so only negative μ has physical meaning. If the ground state energy is ϵ_0, then the limiting value of μ is ϵ_0 instead. □

(e) From the condition $n\lambda_T(T_c)^d = g_{d/2}(1)$, derive the expression for T_c as $k_B T_c = \frac{4\pi}{\zeta(d/2)^{2/d}} \frac{\hbar^2 n^{2/d}}{2m} = \frac{4\pi k_B T_*}{\zeta(d/2)^{2/d}}$, valid for $d > 2$, and $T_c = 6.625 T_*$ in 3D, as given in the notes.

Solution.

By definition,

$$\lambda(T) = \left(\frac{2\pi\hbar^2}{mk_B T} \right)^{1/2}. \tag{2.10}$$

Thus,

$$\zeta(d/2) = n\lambda^d(T_c) = n \left(\frac{2\pi\hbar^2}{mk_B T_c} \right)^{d/2}. \tag{2.11}$$

Inverting, we can write

$$k_B T_c = \frac{2\pi\hbar^2 n^{2/d}}{m\zeta^{2/d}(d/2)} = \frac{4\pi}{\zeta^{2/d}(d/2)} \frac{\hbar^2 n^{2/d}}{2m} = \frac{4\pi}{\zeta^{2/d}(d/2)} k_B T_*. \tag{2.12}$$

For $d = 3$, we can evaluate the prefactor $4\pi/\zeta^{2/3}(3/2) = 6.625$, as given in the lecture notes. □

(f) As discussed at length in the lecture, for $T < T_c$ the condensation density $n_0(T)$ becomes nonzero and growing with decreasing T toward the total density n at $T = 0$. Starting with Eq. 35 in the lecture notes, $n = n_0(T) + \int \frac{d^d k}{(2\pi)^d} \frac{1}{e^{\beta(\epsilon_{\mathbf{k}} - \mu)} - 1}$, derive the temperature dependence of $n_0(T)$ for $T < T_c$ given in the notes, $n_0(T) = n \left[1 - \left(\frac{T}{T_c} \right)^{d/2} \right]$,

Hint: (i) What is the value of μ for $T < T_c$ that we are exploring here? (ii) This significantly simplifies "excitations" of the number equation above (Eq. 35 in notes), as one can change variables and scale T out of the integral. (iii) Note that the value of this last integral at T_c allows us to eliminate the complicated integral and replace it by a power of T_c, thereby giving the desired simple expression for $n_0(T)$.

Solution.

For $T < T_c$, $\mu \approx 0$. Thus, the integration simplifies to

$$\begin{aligned} n &= n_0 + \frac{1}{(2\pi)^d} \int_0^\infty dk \frac{k^{d-1}}{e^{\beta\epsilon} - 1} \\ &= n_0 + \frac{1}{(2\pi)^d} \left(\frac{2m}{\hbar^2}\right)^{d/2} \frac{\pi^{d/2}}{\Gamma(d/2)} \int_0^\infty d\epsilon \frac{\epsilon^{d/2-1}}{e^{\beta\epsilon} - 1} \\ &= n_0 + \frac{1}{\lambda^d(T)} g_{d/2}(1) \\ &= n_0 + n\left(\frac{\lambda(T_c)}{\lambda(T)}\right)^d \\ &= n_0 + n\left(\frac{T}{T_c}\right)^{d/2}. \end{aligned} \tag{2.13}$$

Thus, as desired,

$$n_0 = n\left[1 - \left(\frac{T}{T_c}\right)^{d/2}\right]. \tag{2.14}$$

□

(g) Show that below but close to T_c, the condensate density grows as $n_0(T) \sim T_c - T$.

Solution.

Let $x = T/T_c$, then by a Taylor expansion around $x = 1$,

$$n_0 \approx n_0(x = 1) + \left.\frac{\partial n_0}{\partial x}\right|_{x=1} (x - 1) = -n\frac{d}{2}1^{d/2-1}(x - 1) = \frac{nd}{2T_c}(T_c - T) \sim T_c - T. \tag{2.15}$$

□

(h) Focusing on low temperatures, $T \ll T_c$, derive the power-law excitation energy $E(T) \sim T^{d/2+1}$ and the corresponding heat capacity $C_v(T) \sim T^{d/2}$ quoted in the lecture notes.

Solution.

From the result of part (a), at low temperatures, $\mu \approx 0 \to z \to 1$ and

$$\frac{E}{V} \approx \frac{d}{2}\frac{k_B T}{\lambda_T^d} g_{d/2+1}(1) = \frac{d}{2}\zeta(d/2 + 1)\frac{k_B T}{\lambda_T^d}. \tag{2.16}$$

Since $\lambda_T^d \sim T^{-d/2}$, it then follows that $E \sim T^{d/2+1}$ and $C_v = \partial E/\partial T \sim T^{d/2}$. □

***Problem* 3** (Bose gas in a harmonic potential)**:** Consider a gas of noninteracting *bosonic* atoms in a 3-dimensional *harmonic* potential $V(x,y) = \frac{1}{2}m\omega_0^2 r^2$, as now is routinely done in JILA and other laboratories around the world (physically the harmonic potential is typically either optical or magnetic trap). Let us repeat our in-class and above analysis (for the box with periodic boundary conditions) for this harmonic potential.

(a) Write down the singe-particle energies for this potential.

Solution.

The single-particle Hamiltonian is

$$\mathcal{H} = \left[\frac{\mathbf{p}^2}{2m} + \frac{1}{2}m\omega_0^2\mathbf{r}^2 - \frac{3}{2}\hbar\omega_0\right], \tag{3.1}$$

which has the energy eigenvalues

$$\epsilon_\alpha = \hbar\omega_0(n_x + n_y + n_z), \tag{3.2}$$

where $\alpha_{\mathbf{n}} = (n_x, n_y, n_z)$. □

(b) Use the above result and general thermodynamic analysis (e.g., from lectures) of the Bose gas to write down the N equation as sum over oscillator single particle quantum states $\alpha_{\mathbf{n}} = (n_x, n_y, n_z)$ in 3 dimensions. (For concreteness use the definition of the Hamiltonian such that the ground state single-particle energy in the trap is at zero, i.e., subtract zero-point energy).

Solution.

For bosons, the occupation density is

$$n_\alpha = \frac{1}{e^{\beta(\epsilon_\alpha - \mu)} - 1}. \tag{3.3}$$

Thus,

$$N = \sum_\alpha n_\alpha = \sum_{\mathbf{n}} \left[e^{\beta[\hbar\omega_0(n_x+n_y+n_z)-\mu]} - 1\right]^{-1}. \tag{3.4}$$

□

(c) In the limit of small trap frequency $\hbar\omega_0 \ll k_B T_c$, neglecting the discreteness of $\mathbf{n}$ allows you to replace 3-dimensional sum over $\mathbf{n}$ by 3-dimensional integrals over energies $\epsilon_x, \epsilon_y, \epsilon_z$ (keeping track of the trivial rescaling change of variables) in analogy with what we did for bosons in a box. Your expression for N will again involve the $g_\nu(z)$ function.

Solution.

For $\hbar\omega_0 \ll k_B T_c$, $\sum_{\mathbf{n}} \mapsto \int dn_x dn_y dn_z = \int \frac{d\epsilon_x d\epsilon_y d\epsilon_z}{(\hbar\omega_0)^3}$ and we can write

$$N = \int \frac{d\epsilon_x d\epsilon_y d\epsilon_z}{(\hbar\omega_0)^3} \left[e^{\beta(\epsilon_x+\epsilon_y+\epsilon_z-\mu)} - 1\right]^{-1}. \tag{3.5}$$

The density of states $\mathcal{D}(\epsilon)$ for a given total energy $\epsilon = \epsilon_x + \epsilon_y + \epsilon_z$ is

$$\mathcal{D}(\epsilon) \approx \frac{1}{2}\frac{\epsilon^2}{(\hbar\omega_0)^3}, \tag{3.6}$$

at large ϵ. Thus,

$$\begin{aligned} N &\approx \frac{1}{2}\left(\frac{k_BT}{\hbar\omega_0}\right)^3 \int dx \frac{x^2}{e^x z^{-1} - 1} \qquad (x = \beta\epsilon) \\ &= \frac{1}{2}\left(\frac{k_BT}{\hbar\omega_0}\right)^3 \Gamma(3) g_3(z) \\ &= \left(\frac{k_BT}{\hbar\omega_0}\right)^3 g_3(z). \end{aligned} \tag{3.7}$$

□

(d) Repeat similar calculations for the pressure $P(z)$ and energy $E(z)$, both obtained from $\mathcal{Z}$ and related to the same $g_\nu(z)$ function. Thus show that $P = aE/V$, deriving the proportionality constant a in 3d.

Hint: (i) Recall that degeneracy of a 3d oscillator states at energy $\hbar\omega n$ is $\rho(n) = (1/2)(n+1)(n+2) \approx (1/2)n^2$ for large n, much like $\int dp_x dp_y dp_z \ldots = \text{const.} \int dp p^2 \ldots = \text{const} \int d\epsilon \epsilon^{1/2}$. (ii) The pressure comes from the $\ln\mathcal{Z}$, which will gie an integral over $\mathbf{k}$ of a logarithm. After converting to a 1d radial integral, use integration by parts to make progress to express it in terms of a $g_\nu(z)$ function.

Solution.

First, we calculate the free energy

$$\begin{aligned} \mathcal{F} &= k_BT \sum_{\mathbf{n}} \ln\left[1 - e^{-\beta(\epsilon_\alpha - \mu)}\right] \\ &= k_BT \int \frac{d\epsilon_x d\epsilon_y d\epsilon_z}{(\hbar\omega_0)^3} \ln\left[1 - e^{-\beta(\epsilon_x+\epsilon_y+\epsilon_z-\mu)}\right] \\ &\approx k_BT \frac{1}{2}\int d\epsilon \frac{\epsilon^2}{(\hbar\omega_0)^3} \ln\left[1 - e^{-\beta(\epsilon-\mu)}\right] \\ &= \frac{k_BT}{2}\left(\frac{k_BT}{\hbar\omega_0}\right)^3 \int dx x^2 \ln\left[1 - ze^{-x}\right] \\ &= \frac{k_BT}{2}\left(\frac{k_BT}{\hbar\omega_0}\right)^3 \left[\left.\frac{x^3\ln\left(1 - ze^{-x}\right)}{3}\right|_0^\infty - \frac{1}{3}\int_0^\infty dx \frac{x^3}{e^x z^{-1} - 1}\right] \\ &= -\frac{k_BT}{6}\left(\frac{k_BT}{\hbar\omega_0}\right)^3 \Gamma(4) g_4(z) \\ &= -k_BT\left(\frac{k_BT}{\hbar\omega_0}\right)^3 g_4(z). \end{aligned} \tag{3.8}$$

Then it follows that the pressure is

$$P(z) = -\frac{\mathcal{F}}{V} = k_B T \frac{N}{V}\frac{g_4(z)}{g_3(z)} = nk_B T \frac{g_4(z)}{g_3(z)}. \tag{3.9}$$

Also, the energy is

$$\begin{aligned} E(z) &= \frac{\partial(\beta\mathcal{F})}{\partial\beta} \\ &= -\frac{\partial}{\partial\beta}\left[\frac{g_4(z)}{(\beta\hbar\omega_0)^3}\right] \\ &= 3k_B T \frac{g_4(z)}{(\beta\hbar\omega_0)^3} + \frac{\mu z \partial g_4/\partial z}{(\beta\hbar\omega_0)^3} \\ &= 3k_B T \left(\frac{k_B T}{\hbar\omega_0}\right)^3 g_4(z) + \frac{\mu g_3(z)}{(\beta\hbar\omega_0)^3} \\ &\approx 3Nk_B T \frac{g_4(z)}{g_3(z)}, \end{aligned} \tag{3.10}$$

where we have used the recurrence relation $zg_\nu(z)/\partial z = g_{\nu-1}(z)$ provided in the Appendix of Pathria & Beele (2007). Also the second term vanishes as the gas reaches BEC at $\mu = 0$ ($z = 1$). It then follows that

$$P = \frac{1}{3}\frac{E}{V}. \tag{3.11}$$

□

(e) Using above integral expression in N equation above, derive the expression for the BEC condensation critical temperature T_c for such a harmonically trapped 3d Bose gas. *Hint*: Use the special value of μ at T_c that greatly simplifies the integral expression for N. Evaluate the resulting integrals in the N equation by expanding the associated Bose-Einstein distribution in an infinite power series in $e^{-(\epsilon_x+\epsilon_y+\epsilon_z)/k_B T_c}$. Then observe that you can now perform the three exponential $\epsilon_x, \epsilon_y, \epsilon_z$ integrals, leaving a single summation that should be familiar from the definition of the Riemann-zeta function, $\zeta(d)$.

Solution.
As $T/T_c \to 1$, $\mu \to 0$ and we can write

$$
\begin{aligned}
N &= \sum_{\mathbf{n}} \frac{1}{e^{\beta_c(\epsilon_x+\epsilon_y+\epsilon_z)} - 1} && (\beta_c = 1/k_B T_c) \\
&= \left(\frac{k_B T_c}{\hbar\omega_0}\right)^3 \int \frac{du dv dw}{e^{u+v+w} - 1} && (u = \beta\epsilon_x, v = \beta\epsilon_y, w = \beta\epsilon_z) \\
&= \left(\frac{k_B T_c}{\hbar\omega_0}\right)^3 \sum_{n=1}^{\infty} \int_0^\infty \int_0^\infty \int_0^\infty du dv dw e^{-nu} e^{-nv} e^{-nw} \\
&= \left(\frac{k_B T_c}{\hbar\omega_0}\right)^3 \sum_{n=1}^{\infty} \frac{1}{n^3} \\
&= \left(\frac{k_B T_c}{\hbar\omega_0}\right)^3 \zeta(3). && (3.12)
\end{aligned}
$$

We can then invert to find an expression for the critical temperature

$$k_B T_c = \hbar\omega_0 \left(\frac{N}{\zeta(3)}\right)^{1/3}. \tag{3.13}$$

□

(f) Straightforwardly generalize this result for T_c to d dimensions and note that in a harmonic trap there is indeed nonzero T_c, i.e., BEC even in $d = 2$, unlike the box potential.

Solution.
For d dimensions, we can write

$$k_B T_c = \hbar\omega_0 \left(\frac{N}{\zeta(d)}\right)^{1/d}. \tag{3.14}$$

This expression diverges for $d \leq 1$. Thus, even in $d = 2$, there is still a finite T_c. □

(g) For $T < T_c$ derive the growth of the condensate $N_0(T)$ with reduced T.

Solution.
For $T < T_c$, we write

$$
\begin{aligned}
N &= N_0(T) + \int \frac{d\epsilon_x d\epsilon_y d\epsilon_z}{(\hbar\omega_0)^3} \frac{1}{e^{\beta(\epsilon_x+\epsilon_y+\epsilon_z)} - 1} \\
&= N_0(T) + \left(\frac{k_B T}{\hbar\omega_0}\right)^3 \zeta(3) && \text{(formally the same integral as in part (e))} \\
&= N_0(T) + N\left(\frac{T}{T_c}\right)^3. && (3.15)
\end{aligned}
$$

Then, we get

$$N_0(T) = N\left[1 - \left(\frac{T}{T_c}\right)^3\right]. \tag{3.16}$$

□

(h) Focusing on low temperatures, $T \ll T_c$, following the ideas for the bosons in a box, and thermodynamic limit analysis above, derive the power-law exitation energy $E(T) \sim T^{\alpha_1}$ and the corresponding heat capacity $C_V(T) \sim T^{\alpha_2}$, finding α_1, α_2.

Solution.

From part (d), at low temperatures ($T \ll T_c$), $z \to 1$ and

$$E \to 3Nk_BT\frac{\zeta(4)}{\zeta(3)}. \tag{3.17}$$

However, recall that $N \sim T^3$ from part (c). Thus, $E \sim T^4$ and therefore $C_v \sim T^3$. In other words, $\alpha_1 = 4$, and $\alpha_2 = 3$. □

***Problem* 4** (Black-body radiation)**:** As discussed in the lecture, there are two key differences between atomic Bose gas and a gas of photons. These are (1) the chemical potential $\mu = 0$ (since unlike atoms, photons are not conserved) and single-particle dispersion $\epsilon_k = \hbar ck$ (photon are ultra-relativistic particles) for the latter. Let us apply above analysis to the photon gas in a box (with periodic boundary conditions) to fill in some of the details of the results quoted in the lecture.

(a) Write down a formal expression (in terms of an integral over $\mathbf{k}$) for the total energy $E(T)$ of black-body photons in a 3d box. Without evaluating it, but simply approximating the Bose-Einstein distribution for low frequencies, show that for the range of frequencies $0 < \hbar\omega_k \ll k_B T$, the expression is given by equipartition of energy per photon mode.

Solution.

By definition, the grand canonical partition function is

$$\mathcal{Z} = \prod_{\mathbf{k}} \left[\frac{1}{1 - e^{-\beta\hbar\omega_k}} \right]^2. \tag{4.1}$$

Thus, the total energy is

$$E = -\frac{\partial(\ln \mathcal{Z})}{\partial \beta} = \sum_{\mathbf{k}} \frac{2\hbar\omega_k}{e^{\beta\hbar\omega_k} - 1}. \tag{4.2}$$

Now, for $x = \beta\hbar\omega_k \ll 1$ ($\hbar\omega_k \ll k_B T$), the Bose-Einstein distribution function $n_B = [e^{\beta\hbar\omega_k} - 1]^{-1} \approx 1/x = k_B T/\hbar\omega_k$. Thus, the energy becomes

$$E = 2N k_B T, \tag{4.3}$$

where $N = \sum_{\mathbf{k}} 1$. Thus, the energy follows the equipartition theorem for all photon modes $\mathbf{k}$. $\square$

(b) Calculate the total energy $E(T)$ of black-body photons in a 3d box of volume V and the corresponding heat capacity $C_v(T)$, without above approximation and note that up to a numerical prefactor it gives the same result, as noted in the lectures.

Solution.

Going into the continuum limit $L \to \infty$, we calculate

$$\begin{aligned}
E &= \frac{V}{(2\pi)^3} \int d^3k \frac{2\hbar\omega_k}{e^{\beta\hbar\omega_k} - 1} \\
&= \frac{V}{8\pi^3} 4\pi \int_0^\infty dk k^2 \frac{\hbar\omega_k}{e^{\beta\hbar\omega_k} - 1} \\
&= \frac{V}{\pi^2} \frac{1}{\hbar^2 c^3} \int_0^\infty d\omega \frac{(\hbar\omega)^3}{e^{\beta\hbar\omega} - 1} && (ck = \omega) \\
&= \frac{V\pi^2}{15(\hbar c)^3} (k_B T)^4, && (4.4)
\end{aligned}$$

where we have evaluated the last integral with Mathematica. This expression follows Stefan-Boltzmann Law, as expected. Up to a prefactor $(k_BT/\hbar c)^3$, this gives the same result as part (a). Also, the heat capacity is

$$C_v = \frac{\partial E}{\partial T} = V\frac{4\pi^2 k_B^4}{15(\hbar c)^3}T^3 = 16\frac{\sigma V}{c}T^3. \tag{4.5}$$

□

(c) How does these results generalize in d-dimensions?

Solution.
In d dimensions, $\int d^dk = \int_0^\infty S_d k^{d-1}$. Thus, the integration in (4.4) is

$$E \sim \int_0^\infty d\omega \frac{(\hbar\omega)^d}{e^{\beta\hbar\omega}-1} \sim \beta^{-(d+1)} \sim T^{d+1}, \tag{4.6}$$

and $C_V \sim T^d$ follows immediately. □

(d) Derive the energy spectral density $u(\omega)$ defined by $E = \int d\omega n(\omega)$ for d-dimensions, and find its limits at low and high frequencies, $\hbar\omega \ll k_BT$ (classical) and $\hbar\omega \gg k_BT$ (quantum), respectively.

Solution.
Now, we redo the previous part more carefully. First, let $\sum_{\mathbf{k}} \to (L/2\pi)^d \int d^dk$ as $L \to \infty$. We get

$$\begin{aligned}\frac{E}{V} &= \frac{1}{(2\pi)^d}\int d^dk \frac{2\hbar\omega_k}{e^{\beta\hbar\omega_k}-1} \\ &= \frac{2S_d}{(2\pi)^d}\int_0^\infty dk k^{d-1}\frac{\hbar\omega_k}{e^{\beta\hbar\omega_k}-1} \\ &= \frac{2S_d}{(2\pi)^d\hbar^{d-1}c^d}\int_0^\infty d\omega\frac{(\hbar\omega)^d}{e^{\beta\hbar\omega}-1}.\end{aligned} \tag{4.7}$$

Reading off of this, the energy spectral density in d dimensions is

$$u(\omega) = \frac{2S_d}{(2\pi)^d\hbar^{d-1}c^d}\frac{(\hbar\omega)^d}{e^{\beta\hbar\omega}-1} = \frac{(k_BT)^d}{\Gamma(d/2)2^{d-2}\pi^{d/2}\hbar^{d-1}c^d}\frac{(\beta\hbar\omega)^d}{e^{\beta\hbar\omega}-1}. \tag{4.8}$$

At low frequency, $e^{\beta\hbar\omega}-1 \approx \beta\hbar\omega$ and $u(\omega)$ grows as $(\beta\hbar\omega)^{d-1}$. At high frequency, the exponential term dominates over unity and thus $u(\omega) \sim (\beta\hbar\omega)^d e^{-\beta\hbar\omega}$. So u decays exponentially. □

(e) Derive the peak frequency ω_p of $u(\omega)$ in terms of the temperature of the black-body in 3d. Estimate that frequency for the Sun and for yourself (treating each as a black-body). How do you explain the "coincidence" that this peak frequency for the Sun falls into the visible range for our eyes?

Solution.

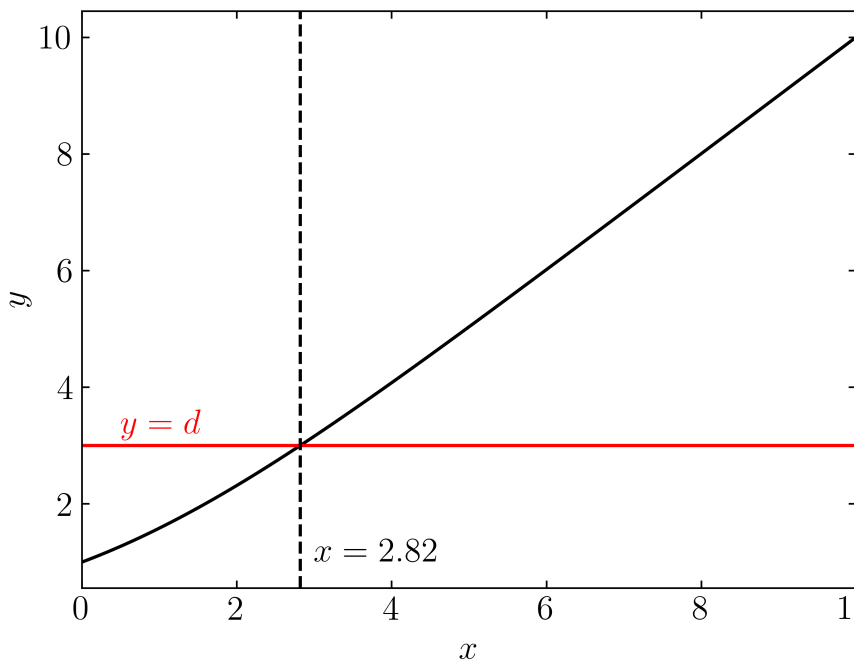
The peak frequency ω_p satisfies

$$\frac{\partial u}{\partial \omega} \sim \frac{d(\beta\hbar\omega)^{d-1}}{e^{\beta\hbar\omega}-1} - \frac{(\beta\hbar\omega)^d e^{\beta\hbar\omega}}{(e^{\beta\hbar\omega}-1)^2} = 0. \tag{4.9}$$

The solution to this is a transcendental equation

$$d = y(x) = \frac{x}{1-e^{-x}}, \tag{4.10}$$

where $x = \beta\hbar\omega$. We can find the solution graphically for $d = 3$.



From the graph above, the root is at $x \approx 2.82$. Thus, the peak frequency is

$$f_p = \frac{\omega_p}{2\pi} = \frac{2.84}{2\pi}\frac{k_B T}{\hbar}. \tag{4.11}$$

For the average human body temperature, $T_{\text{human}} = 310\,\text{K}$, leading to $f_p \approx 18\,\text{Hz}$. For the average solar surface temperature $T_{\text{sun}} = 5772\,\text{K}$, the peak frequency is $f_p \approx 340\,\text{THz}$. This is very close to the visible range from $\sim 400 - 790\,\text{THz}$, which makes sense because the human eyes should be adapted to recognize the only prominent source of radiation in the solar system, which is the Sun. $\square$

(f) Derive the relation between the pressure $P(T)$ (using $\mathcal{Z}$) and the energy $E(T)$, verifying the characteristic result $P = (1/d)E/V$.

Hint: (i) Note the very close relation of this problem to that of finite temperature excitations above an atomic condensate. (ii) A d-dimensional photon has $d-1$ polarizations (that you can take to be degenerate) tranverse to the propagation wavevector **k**. (iii) After scaling out T the integral can be reduced to a pure number that you can compute via e.g., Mathematica. (iv) Refer to Hints in 3(d).

Solution.
First, we calculate the free energy

$$\begin{aligned}
\mathcal{F} &= -k_B T \ln \mathcal{Z} \\
&= 2k_B T \sum_{\mathbf{k}} \ln\left(1 - e^{-\beta\hbar\omega}\right) \\
&= 2k_B T \frac{V S_d}{(2\pi)^d} \int_0^\infty dk k^{d-1} \ln\left(1 - e^{-\beta\hbar\omega}\right) \\
&= V k_B T \frac{2S_d}{(2\pi c)^d} \int_0^\infty d\omega \omega^{d-1} \ln\left(1 - e^{-\beta\hbar\omega}\right) \\
&= -V \frac{2S_d \hbar}{d(2\pi\hbar c)^d} \int_0^\infty d\omega \frac{(\hbar\omega)^d}{e^{\beta\hbar\omega} - 1}.
\end{aligned} \tag{4.12}$$

Then, the pressure is

$$P = -\frac{\mathcal{F}}{V} = \frac{2S_d}{(2\pi c)^d \hbar^{d-1}} \int_0^\infty d\omega \frac{(\hbar\omega)^d}{e^{\beta\omega} - 1}. \tag{4.13}$$

Comparing this with (4.7), we can write

$$P = \frac{1}{d}\frac{E}{V}. \tag{4.14}$$

□

***Problem* 5** (Phonons in a Debye solid)**:** As discussed in the lecture, there are only few more differences between acoustic phonons and black-body phonons. These are (1) while acoustic phonon dispersion ω_k is linear in k near $k = 0$, just like that of a photon, with speed of light replaced by speed of sound, more generally phonon dispersion is given by some nonlinear function ω_k. (It is also typically quite anisotropic, depending on $\mathbf{k}$ not just its magnitude k, but this we will neglect). (2) Because phonons are normal modes of vibrations of discrete periodic array of N atoms, there only N normal modes $\mathbf{k}$ and thus there is a maximum value of $\mathbf{k}$ defining the Brillouin Zone of N wavevectors $\mathbf{k}$ values. (3) There are d normal phonon modes per $\mathbf{k}$ rather than $d-1$ of transverse photons. Since phonons are non-conserved excitations, they are also characterized by a $\mu = 0$.

As discussed in the lectures, we approximate true acoustic phonons with a 'toy' model of Debye phonons, taking ω_k to be linear in k throughout, i.e., $v\hbar k$, for $k \le k_{\text{Debye}}$, where the limiting k_{Debye} is determined by the constraint that there are a total of N normal modes (per polarization) in the crystal. Thus, the main crucial difference from the photons is that there is a limiting upper k_{Debye} and equivalently upper Debye frequency, $\omega_{\text{Debye}} = v k_{\text{Debye}}$.

Armed with these facts, we will now fill in some of the details of the results quoted in the lecture.

(a) Starting with the grand-canonical partition function, derive the integral forms (over ω) of the total energy $E(T)$ and the corresponding heat capacity $C_v(T)$ in a d-dimensional isotropic Debye solid.

Solution.

By definition, the grand-canonical partition function is

$$\mathcal{Z} = \sum_{\{n_{\mathbf{k},\alpha}\}} \exp\left[-\beta E_{\{n_{\mathbf{k},\alpha}\}}\right], \tag{5.1}$$

where $E_{\{n_{\mathbf{k},\alpha}\}} = \sum_{\mathbf{k},\alpha} \hbar\omega_{k,\alpha} n_{\mathbf{k},\alpha}$. Then, it follows that

$$\begin{aligned}
\mathcal{Z} &= \sum_{\{n_{\mathbf{k},\alpha}\}} \prod_{\mathbf{k}\in\text{BZ},\alpha} \exp\left(-\beta n_{\mathbf{k},\alpha}\hbar\omega_{k,\alpha}\right) \\
&= \prod_{\mathbf{k}\in\text{BZ},\alpha} \sum_{n_{\mathbf{k},\alpha}=0}^{\infty} \exp\left(-\beta\hbar\omega_{k,\alpha}\right)^{n_{\mathbf{k},\alpha}} \\
&= \prod_{\mathbf{k}\in\text{BZ},\alpha} \frac{1}{1-e^{-\beta\hbar\omega_{k,\alpha}}},
\end{aligned} \tag{5.2}$$

where BZ is the Brillouin Zone for each normal mode α. Now, by definition, the energy is

$$\begin{aligned}
E &= -\frac{\partial(\ln \mathcal{Z})}{\partial\beta} \\
&= \sum_{\mathbf{k}\in\mathrm{BZ},\alpha} \frac{\partial}{\partial\beta} \ln\left(1 - e^{-\beta\hbar\omega_{k,\alpha}}\right) \\
&= \sum_{\mathbf{k}\in\mathrm{BZ},\alpha} \frac{\hbar\omega_{k,\alpha}}{e^{\beta\hbar\omega_{k,\alpha}} - 1}. \\
&= \int d\omega \sum_{\mathbf{k}\in\mathrm{BZ},\alpha} \delta(\omega - \omega_{k,\alpha}) \frac{\hbar\omega}{e^{\beta\hbar\omega} - 1} \\
&= \int d\omega g(\omega) \frac{\hbar\omega}{e^{\beta\hbar\omega} - 1},
\end{aligned} \tag{5.3}$$

where the density of states is

$$\begin{aligned}
g(\omega) &= \sum_{\mathbf{k}\in\mathrm{BZ},\alpha} \delta(\omega - \omega_{k,\alpha}) \\
&= \sum_{\mathbf{k}\in\mathrm{BZ}} \delta(\omega - c_L k) + (d-1) \sum_{\mathbf{k}\in\mathrm{BZ}} \delta(\omega - c_T k) \\
&= V \int_{\mathrm{BZ}} \frac{d^d k}{(2\pi)^d} \left[\delta(\omega - c_L k) + (d-1)\delta(\omega - c_T k)\right] \\
&= V \frac{S_d}{(2\pi)^d} \int_0^{k_D} dk k^{d-1} \left[\frac{1}{c_L}\delta(k - \frac{\omega}{c_L}) + \frac{d-1}{c_T}\delta(k - \frac{\omega}{c_T})\right] \\
&= \frac{V}{\Gamma(d/2) 2^{d-1} \pi^{d/2}} \left(\frac{1}{c_L^d} + \frac{d-1}{c_T^d}\right) \omega^{d-1},
\end{aligned} \tag{5.4}$$

for $\omega < \omega_D$ and zero otherwise. c_T, c_L are the transverse and longitudinal acoustic speed. The constraint for the number of modes is

$$dN = \int g(\omega) d\omega = \frac{V}{\Gamma(d/2) 2^{d-1} \pi^{d/2}} \left(\frac{1}{c_L^d} + \frac{d-1}{c_T^d}\right) \frac{\omega_D^d}{d}. \tag{5.5}$$

Thus, the Debye frequency is determined by

$$\omega_D^d = d^2 \Gamma(d/2) 2^{d-1} \pi^{d/2} \frac{N}{V} \left(\frac{1}{c_L^d} + \frac{d-1}{c_T^d}\right)^{-1}. \tag{5.6}$$

This gives a simplified form for the density of states

$$g(\omega) = d^2 N \frac{\omega^{d-1}}{\omega_D^d}. \tag{5.7}$$

Plugging this in, we get the energy

$$E = \frac{d^2 N}{\hbar^{d-1}\omega_D^d}\int_0^{\omega_D} d\omega \frac{(\hbar\omega)^d}{e^{\beta\hbar\omega}-1}. \tag{5.8}$$

Then, we can also calculate

$$C_V = \frac{\partial E}{\partial T} = \frac{d^2 N k_B \beta^2}{\hbar^{d-1}\omega_D^d}\int_0^{\omega_D} d\omega \frac{(\hbar\omega)^{d+1}e^{\beta\hbar\omega}}{(e^{\beta\hbar\omega}-1)^2}. \tag{5.9}$$

□

(b) Based on your analytic integral expression for $C_v(T)$, argue that (i) for $k_B T \ll \hbar\omega_D$, the result reduces to that of the black-body heat capacity, and in contrast (ii) for $k_B T \gg \hbar\omega_D$, heat capacity crosses over (plateaus to) the equipartition value, as expected. What is the number of degrees of freedom that this gives in d dimensions?

Solution.
Letting $x = \beta\hbar\omega$, the expression for C_v becomes

$$C_v = \frac{d^2 N k_B}{x_D^d}\int_0^{x_D} dx \frac{x^{d+1}e^x}{(e^x-1)^2}, \tag{5.10}$$

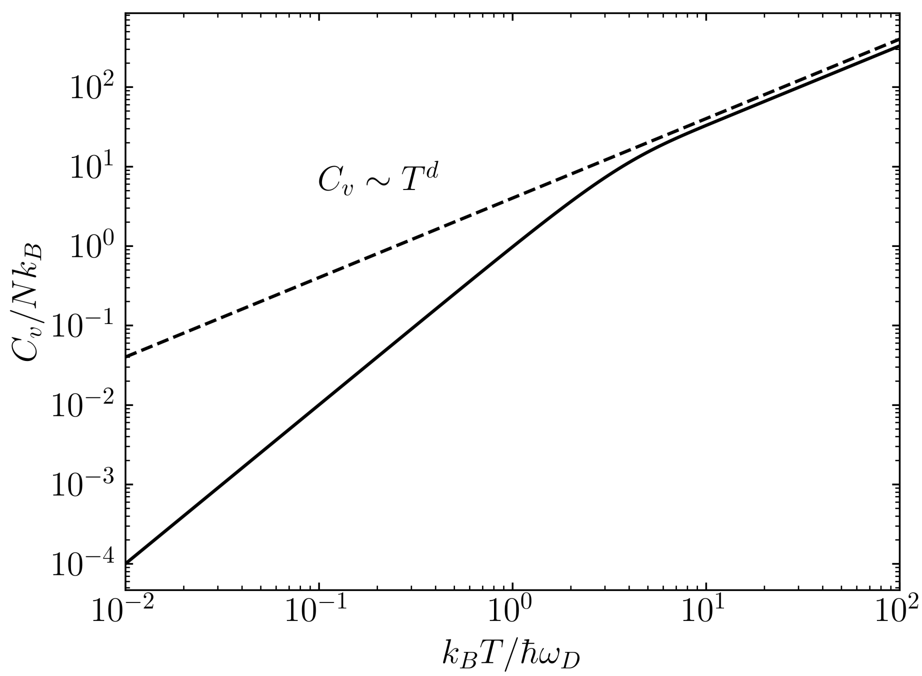
where $x_D = \beta\hbar\omega_D$. For $x_D \to \infty$, the integral converges to some finite value. Thus, $C_v \sim x_D^{-d} \sim T^d$, similar to the black-body result attained in the previous problem. On the other hand, if x_D is small, then the integrand can be expanded to lowest order in x,

$$C_v(x_D \ll 1) \approx \frac{d^2 N k_B}{x_D^d}\int_0^{x_D} dx x^{d-1} = dNk_B, \tag{5.11}$$

resulting in equipartition in dN degrees of freedom. □

(c) Sketch $C_v(T)$ as a function of T for a fixed value of Debye frequency ω_D, paying attention to the behavior of the expression for T relative to $\hbar\omega_D/k_B$. Check your sketch with Mathematica.

Solution.
Below, we plot (5.10) in terms of x.



The transition temperature is a bit higher than $x = 1$, albeit on the same order of magnitude. At low temperature, the system freezes out, while at high temperature, C_v approaches the black-body behaviors. $\square$

***Problem* 6** (Fermi gas thermodynamics: electrons in a metal)**:** In lectures we introduced noninteracting (ideal) Fermi gas in a box (with periodic boundary conditions) and presented many results, some without derivations. Here I will ask you to derive some of the details.

The theory describes thermodynamics of any gas (noninteracting) of N fermionic particles. The most important applications of this theory is to that of the electrons confined inside of a piece of metal. It also describes a neutron star composed of neutrons, as well as trapped fermionic atomic gases, such as e.g., K^{40} as first cooled to degeneracy by Professor Debbie Jin in her seminal work dating back to 1999.

(a) Details of the Fermi distribution function

Starting from the fermionic grand-partition function $\mathcal{Z}$, we wrote don the expression for the expectation value for the occupation of the α single-particle state, namely $\langle n_\alpha \rangle_F = 1/\left[e^{(\epsilon_\alpha-\mu)/k_BT}+1\right]$, the so-called Fermi-Dirac distribution.

(i) Derive $n_F(\epsilon_k)$ from the fermionic grand-partition function $\mathcal{Z}$ for spinless fermions. How does it trivially extend for spin-1/2 electrons in zero magnetic field?

(ii) Plot $n_F(\epsilon_k)$ and its derivative $\partial_{\epsilon_k} n_F(\epsilon_k)$ for fixed positive chemical potential $\mu > 0$ as a function of ϵ_k for a series of k_BT/μ values, covering high (Boltzmann gas) and low (degenerate gas) temperature limits.

(iii) Combine above graphical analysis with analytical examination of $n_F(\epsilon_k)$ in $T \to 0$ limit to show that at $T = 0$, it becomes a step function $\theta(\epsilon_k - \mu)$ at $\mu = \epsilon_F$ and $\partial_\epsilon n_F(\epsilon) = A\delta(\epsilon - \epsilon_F)$ a δ-function, where $\epsilon_F = \mu(T = 0)$. What is the amplitude of A of the δ-function?

Solution.

(i) The energy eigenvalues for spinless fermions are

$$\epsilon_k = \frac{\hbar^2 k^2}{2m}. \tag{6.1}$$

Thus, the FD distribution is

$$n_F = \frac{1}{e^{\beta(\epsilon_k-\mu)}+1} = \frac{1}{e^{\beta(\hbar^2k^2/2m-\mu)}+1}. \tag{6.2}$$

For spin-1/2 electrons, the energy eigenvalues are

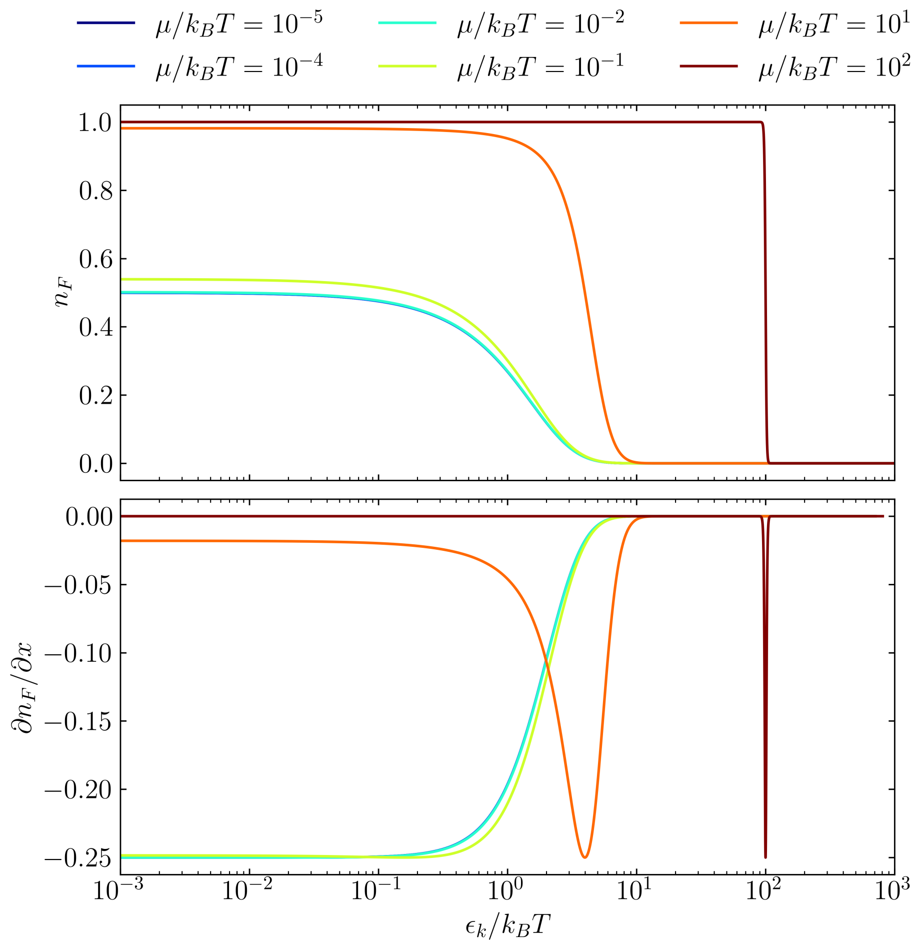
$$\epsilon_k = \frac{\hbar^2 k^2}{2m} + \sigma\mu_B B, \tag{6.3}$$

for $\sigma \in \{1, -1\}$. However, in zero magnetic field, they are the same as the spinless case. Thus, the FD distribution for them is also the same as (6.2).

(ii) The derivative of (6.2) is

$$\frac{\partial n_F}{\partial \epsilon_k} = -\beta \frac{e^{\beta(\epsilon_k-\mu)}}{(e^{\beta(\epsilon-\mu)}+1)^2}. \tag{6.4}$$

Below, we plot n_F (upper pannel) and $\partial n_F/\partial x$ (lower panel) where $x = \beta\epsilon_k$.



(iii) Indeed, n_F becomes a step function $\theta(\epsilon_k - \mu)$, while n_F' becomes a delta function as $T \to 0$. Also, by inspection, at $\mu = \epsilon_k$, we can evaluate

$$\frac{1}{\beta}\frac{\partial n_F}{\partial \epsilon_k} = -\frac{e^{\beta(\epsilon-\mu)}}{(e^{\beta(\epsilon-\mu)}+1)^2} = -\frac{1}{4}. \tag{6.5}$$

Thus, the amplitude of the delta function is $-1/4$. As seen in the second panel, all curves reach minimum at -0.25. □

(b) Zero-temperature Fermi gas analysis

(i) Let's reexamine the number N equation for $T = 0$. Use the above derived $T = 0$ form of the Fermi function to compute the right hand side of the N equation, and thereby derive the relation between the Fermi energy $\epsilon_F(n)$ (upper limit of the energy ϵ integral) and the density n in d dimensions.

Hint: (i) Notice that in this $T = 0$ limit, the step-function of amplitude 1 just corresponds to filling al the lowest energy states $\mathbf{k}$ at single-particle energies $\epsilon_{\mathbf{k}}$ one by one with N fermions (one per $\mathbf{k}$, since we ignore electron spin – think of it as being polarized by a strong external B field and thus only one lowest spin state matters), corresponding to the highest Fermi energy, ϵ_F. (ii) In this imit the integral is trivial exercise in d dimensional calculus, that we already extensively discussed (do the integral over angular variables getting S_d, followed by a simple radial k integral up to k_F). (iii) Check your answer based on dimensional analysis, recalling our discussion of the degeneracy energy $k_B T_*$ in the lecture.

(ii) Calculate the *total* many-body energy $E(n) = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} n_F(\epsilon_{\mathbf{k}})$ as a function of the fermion density in d dimensions. Do it in the thermodynamic limit where the sum over $\mathbf{k}$ can be replaced by appropriate $\mathbf{k}$ integral, as in the number equation problem, above. Check that your answer satisfies the dimensional analysis, and noting that $E(n)$ can be written in terms of n and $\epsilon_F(n)$ derived above.

(iii) What is the equivalent Fermi temperature, $T_F = E_F/k_B$ for electrons in a metal like Sodium, Na? At this energy, what is the velocity of the electron at this kinetic energy? Be amazed at this Pauli principle enforced result, given that the electrons are at zero temperature.

Hint: Atoms in a crystal are typically an Angstrom apart (that's because atoms are about an Angstrom in size as you know from study of the hydrogen atom), with each donating an electron (in Alkali atoms of the first coumn of the periodic table), thereby setting the electron spacing and their corresponding number density. The associated energy is a familiar energy that you all encountered corresponding to an eectron's kinetic eneryg associated with deBroglie wavelength of an Angstrom, thereby not really requiring any further calculations (but you are welcome to put the numbers in to verify the answer).

Solution.

(i) By definition, at $T = 0$, $\mu = \epsilon_F$ and

$$\begin{aligned} N &= \sum_{\mathbf{k}} \theta(\epsilon_k - \epsilon_F) \\ &= \frac{V}{(2\pi)^d} S_d \int_0^{k_F} dk k^{d-1} \\ &= \frac{V}{\Gamma(d/2)(4\pi)^{d/2}} \left(\frac{2m}{\hbar^2}\right)^{d/2} \int_0^{\epsilon_F} d\epsilon \epsilon^{d/2-1} \\ &= \frac{2}{d} \frac{V}{\Gamma(d/2)} \frac{1}{\lambda^d} \left(\frac{\epsilon_F}{k_B T}\right)^{d/2}. \end{aligned} \tag{6.6}$$

We can then invert to write

$$\epsilon_F(n) = k_B T \Big[\Gamma(d/2+1)(n\lambda^d)\Big]^{2/d}. \tag{6.7}$$

(ii) Similarly, we can also calculate

$$
\begin{aligned}
E(n) &= \frac{V}{(2\pi)^d}\int d^d k \epsilon_k \theta(\epsilon_k - \epsilon_F) \\
&= \frac{V}{(2\pi)^d}\frac{\pi^{d/2}}{\Gamma(d/2)}\left(\frac{2m}{\hbar^2}\right)^{d/2}\int_0^{\epsilon_F} d\epsilon \epsilon^{d/2} \\
&= \frac{V}{(d/2+1)\Gamma(d/2)}\frac{1}{\lambda^d}\left(\frac{\epsilon_F}{k_B T}\right)^{d/2}\epsilon_F \\
&= \frac{d/2}{d/2+1}N\epsilon_F \\
&= \frac{d}{d+2}Nk_B T\Big[\Gamma(d/2+1)(n\lambda^d)\Big]^{2/d}.
\end{aligned}
\tag{6.8}
$$

The dimensions make sense.

(iii) From Google, the Fermi energy of sodium is 3.24 eV. Thus, the equivalent Fermi temperature is $T_F \approx 3.76 \times 10^4$ K, and the velocity of electrons at this temperature is $v = \sqrt{2T/m_e} \approx 1.1 \times 10^6$ m/s. □

(c) Nonzero-temperature Fermi gas analysis

For electron as we discussed at high temperature $T \gg T_*$, the gas is nondegenerate and its phenomenology is that of the Boltzmann gas, with e.g., $\mu(T) \sim -T \ln T$, independent of whether the particles are fermions or bosons. However, in contrast to bosons, for fermions the chemical potential crosses zero and becomes positive in the degenerate, low-temperature regime $T < T_*$, at $T = 0$ saturating at a value that is named Fermi energy, $\epsilon_F = \hbar^2 k_F^2/2m$, where $\hbar k_F$ is the so-called Fermi momentum defined by above expression, corresponding to the Fermi wavevector k_F, denoting the highest momentum state occupied at $T = 0$. This behavior is valid for Fermi gas in any dimension, but is particularly simple to work out in two dimensions (2d).

(i) Write down the number equation N in 2d and carry out the momentum integral exactly, thereby finding $\mu(T, n)$.

Hint: It is convenient to change variables to $x = \beta(\epsilon_k - \mu)$ and then rewrite the resulting integrand in terms of e^{-x}, which gives a nice Jacobian for a straightforward exact integration.

(ii) Analyze the resulting analytical expression $\mu(T, n)$ for high- and low-temperatures limits with respect to T_* (i.e., the Fermi temperature $T_F = \epsilon_F/k_B$), recovering the expected Boltzmann gas behavior and asymptotic temperature independent Fermi energy $\epsilon_F(n)$ value as a function of the density, found above.

(iii) Plot this 2d result for $\mu(T, n)$ for high and low temperatures as a function of T.

(iv) At low temperature $T \ll T_F$ compute $E(T, n)$ nd the corresponding heat capacity $C_V(T, n)$, noting the expected failure of the equipartition.

Hint: Do this only as the lowest order in T/T_F correction to the zero-temperature total energy $E(n)$ computed above.

Solution.

(i) By definition, the exact number equation is

$$\begin{aligned} N &= \sum_{\mathbf{k}} \frac{1}{e^{\beta(\epsilon_k-\mu)}} \\ &= \frac{L^2}{(2\pi)^2} 2\pi \int_0^\infty dk \frac{k}{e^{\beta(\epsilon-\mu)}+1} \qquad (6.9) \\ &= \frac{L^2}{2\pi}\frac{m}{\hbar^2} \int_0^\infty \frac{d\epsilon}{e^{\beta(\epsilon-\mu)}+1} \\ &= \left(\frac{L}{\lambda}\right)^2 \int_{-\mu\beta}^\infty \frac{dx}{e^x+1} \\ &= \left(\frac{L}{\lambda}\right)^2 \sum_{n=1}^\infty (-1)^{n-1} \int_{-\mu\beta}^\infty dx e^{-nx} \\ &= \left(\frac{L}{\lambda}\right)^2 \sum_{n=1}^\infty (-1)^{n-1} \frac{e^{n\mu\beta}}{n} \\ &= \left(\frac{L}{\lambda}\right)^2 \ln\left(1+e^{\mu\beta}\right). \qquad (6.10) \end{aligned}$$

Inverting this yields

$$\mu(T,n) = k_B T \ln\left(e^{n\lambda^2}-1\right) = k_B T \ln\left(e^{\epsilon_F/k_BT}-1\right), \qquad (6.11)$$

where $n = N/A$ and we have used previous result (6.7). Letting $\epsilon_F = k_B T_*$, the chemical potential becomes

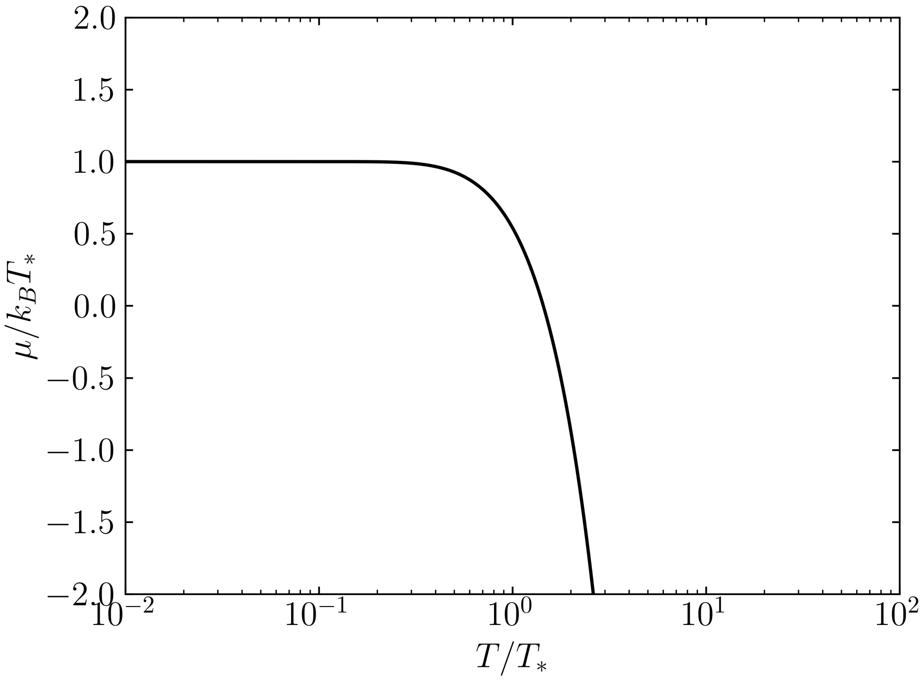
$$\frac{\mu}{k_B T_*} = \frac{T}{T_*} \ln\left(e^{T_*/T}-1\right). \qquad (6.12)$$

(ii) For large temperature $T \gg T_*$, $e^{T_*/T} - 1 \approx T_*/T$ and we recover the classical Boltzmann gas result

$$\frac{\mu}{k_B T_*} \approx -\frac{T}{T_*} \ln\left(\frac{T}{T_*}\right). \qquad (6.13)$$

In the opposite end, at low temperature $T \ll T_*$, the exponential term dominates unity and the chemical potential $\mu/k_B T_* \approx (T/T_*) \ln\left(e^{T_*/T}\right) = 1$, which is consistent with $\mu(T=0) = \epsilon_F$.

(iii) Below, the plotted chemical potential saturates as expected.



(iv) At $T \ll T_*$, $\mu = \epsilon_F$ and we can calculate

$$
\begin{aligned}
E(n) &= \sum_{\mathbf{k}} \frac{\epsilon_k}{e^{\beta(\epsilon_k - \epsilon_F)} + 1} \\
&\approx \frac{L^2 m}{2\pi\hbar^2} \int_0^\infty \epsilon e^{\beta(\epsilon - \epsilon_F)} d\epsilon \\
&= \left(\frac{L}{\lambda}\right)^2 k_B T e^{-\beta\epsilon_F} \\
&\approx \left(\frac{L}{\lambda}\right)^2 k_B T,
\end{aligned}
\tag{6.14}
$$

to the lowest order. It then follows that $C_v = (L/\lambda)^2 k_B$, which doesn't satisfy equipartition. $\square$