

5 Quantum Statistics : Worked Examples

(5.1) For a system of noninteracting $S = 0$ bosons obeying the dispersion $\varepsilon(\mathbf{k}) = \hbar v|\mathbf{k}|$.

- Find the density of states per unit volume $g(\varepsilon)$.
- Determine the critical temperature for Bose-Einstein condensation in three dimensions.
- Find the condensate fraction n_0/n for $T < T_c$.
- For this dispersion, is there a finite transition temperature in $d = 2$ dimensions? If not, explain why. If so, compute $T_c^{(d=2)}$.

Solution :

(a) The density of states in d dimensions is

$$g(\varepsilon) = \int \frac{d^d k}{(2\pi)^d} \delta(\varepsilon - \hbar v k) = \frac{\Omega_d}{(2\pi)^d} \frac{\varepsilon^{d-1}}{(\hbar v)^d} .$$

(b) The condition for $T = T_c$ is to write $n = n(T_c, \mu = 0)$:

$$n = \int_0^\infty d\varepsilon \frac{g(\varepsilon)}{e^{\varepsilon/k_B T_c} - 1} = \frac{1}{2\pi^2 (\hbar v)^3} \int_0^\infty d\varepsilon \frac{\varepsilon^2}{e^{\varepsilon/k_B T_c} - 1} = \frac{\zeta(3)}{\pi^2} \left(\frac{k_B T_c}{\hbar v} \right)^3 .$$

Thus,

$$k_B T_c = \left(\frac{\pi^2}{\zeta(3)} \right)^{1/3} \hbar v n^{1/3} .$$

(c) For $T < T_c$, we have

$$n = n_0 + \frac{\zeta(3)}{\pi^2} \left(\frac{k_B T}{\hbar v} \right)^3 \quad \Rightarrow \quad \frac{n_0}{n} = 1 - \left(\frac{T}{T_c(n)} \right)^3 .$$

(d) In $d = 2$ we have

$$n = \frac{1}{2\pi (\hbar v)^2} \int_0^\infty d\varepsilon \frac{\varepsilon}{e^{\varepsilon/k_B T_c} - 1} = \frac{\zeta(2)}{2\pi} \left(\frac{k_B T_c}{\hbar v} \right)^2 \quad \Rightarrow \quad k_B T_c^{(d=2)} = \hbar v \sqrt{\frac{2\pi n}{\zeta(2)}} .$$

(5.2) Consider a three-dimensional Fermi gas of $S = \frac{1}{2}$ particles obeying the dispersion relation $\varepsilon(\mathbf{k}) = A |\mathbf{k}|^4$.

- (a) Compute the density of states $g(\varepsilon)$.
- (b) Compute the molar heat capacity at low temperatures.
- (c) Compute the lowest order nontrivial temperature dependence for $\mu(T)$ at low temperatures. *I.e.* compute the $\mathcal{O}(T^2)$ term in $\mu(T)$.

Solution :

(a) The density of states in $d = 3$, with $g = 2S + 1 = 2$, is given by

$$g(\varepsilon) = \frac{1}{\pi^2} \int_0^\infty dk k^2 \delta(\varepsilon - \varepsilon(k)) = \frac{1}{\pi^2} k^2(\varepsilon) \frac{dk}{d\varepsilon} \Big|_{k=(\varepsilon/A)^{1/4}} = \frac{\varepsilon^{-1/4}}{4\pi^2 A^{3/4}} \quad .$$

(b) The molar heat capacity is

$$c_V = \frac{\pi^2}{3n} R g(\varepsilon_F) k_B T = \frac{\pi^2 R}{4} \cdot \frac{k_B T}{\varepsilon_F} \quad ,$$

where $\varepsilon_F = \hbar^2 k_F^2 / 2m$ can be expressed in terms of the density using $k_F = (3\pi^2 n)^{1/3}$, which is valid for any isotropic dispersion in $d = 3$. In deriving this formula we had to express the density n , which enters in the denominator in the above expression, in terms of ε_F . But this is easy:

$$n = \int_0^{\varepsilon_F} d\varepsilon g(\varepsilon) = \frac{1}{3\pi^2} \left(\frac{\varepsilon_F}{A} \right)^{3/4} \quad .$$

(c) We have (lecture notes, ch. 5)

$$\delta\mu = -\frac{\pi^2}{6} (k_B T)^2 \frac{g'(\varepsilon_F)}{g(\varepsilon_F)} = \frac{\pi^2}{24} \cdot \frac{(k_B T)^2}{\varepsilon_F} \quad .$$

Thus,

$$\mu(n, T) = \varepsilon_F(n) + \frac{\pi^2}{24} \cdot \frac{(k_B T)^2}{\varepsilon_F(n)} + \mathcal{O}(T^4) \quad ,$$

where $\varepsilon_F(n) = A (3\pi^2 n)^{4/3}$.

(5.3) A bosonic gas is known to have a power law density of states $g(\varepsilon) = A \varepsilon^\sigma$ per unit volume, where σ is a real number.

- (a) Experimentalists measure T_c as a function of the number density n and make a log-log plot of their results. They find a beautiful straight line with slope $\frac{3}{7}$. That is, $T_c(n) \propto n^{3/7}$. Assuming the phase transition they observe is an ideal Bose-Einstein condensation, find the value of σ .
- (b) For $T < T_c$, find the heat capacity C_V .
- (c) For $T > T_c$, find an expression for $p(T, z)$, where $z = e^{\beta\mu}$ is the fugacity. Recall the definition of the polylogarithm (or generalized Riemann zeta function)¹,

$$\text{Li}_q(z) \equiv \frac{1}{\Gamma(q)} \int_0^\infty dt \frac{t^{q-1}}{z^{-1}e^t - 1} = \sum_{n=1}^{\infty} \frac{z^n}{n^q} \quad ,$$

where $\Gamma(q) = \int_0^\infty dt t^{q-1} e^{-t}$ is the Gamma function.

- (d) If these particles were fermions rather than bosons, find (i) the Fermi energy $\varepsilon_F(n)$ and (ii) the pressure $p(n)$ as functions of the density n at $T = 0$.

Solution :

- (a) At $T = T_c$, we have $\mu = 0$ and $n_0 = 0$, hence

$$n = \int_{-\infty}^{\infty} d\varepsilon \frac{g(\varepsilon)}{e^{\varepsilon/k_B T_c} - 1} = \Gamma(1 + \sigma) \zeta(1 + \sigma) A (k_B T_c)^{1+\sigma} \quad .$$

Thus, $T_c \propto n^{\frac{1}{1+\sigma}} = n^{3/7}$ which means $\sigma = \frac{4}{3}$.

- (b) For $T < T_c$ we have $\mu = 0$, but the condensate carries no energy. Thus,

$$\begin{aligned} E &= V \int_{-\infty}^{\infty} d\varepsilon \frac{\varepsilon g(\varepsilon)}{e^{\varepsilon/k_B T} - 1} = \Gamma(2 + \sigma) \zeta(2 + \sigma) A (k_B T)^{2+\sigma} \\ &= \Gamma\left(\frac{10}{3}\right) \zeta\left(\frac{10}{3}\right) A (k_B T)^{10/3} \quad . \end{aligned}$$

Thus,

$$C_V = \Gamma\left(\frac{13}{3}\right) \zeta\left(\frac{10}{3}\right) A (k_B T)^{7/3} \quad ,$$

where we have used $z \Gamma(z) = \Gamma(z + 1)$.

- (c) The pressure is $p = -\Omega/V$, which is

$$\begin{aligned} p(T, z) &= -k_B T \int_{-\infty}^{\infty} d\varepsilon g(\varepsilon) \ln(1 - z e^{-\varepsilon/k_B T}) = -A k_B T \int_0^\infty d\varepsilon \varepsilon^\sigma \ln(1 - z e^{-\varepsilon/k_B T}) \\ &= \frac{A}{1 + \sigma} \int_0^\infty d\varepsilon \frac{\varepsilon^{1+\sigma}}{z^{-1} e^{\varepsilon/k_B T} - 1} = \Gamma(1 + \sigma) A (k_B T)^{2+\sigma} \text{Li}_{2+\sigma}(z) \\ &= \Gamma\left(\frac{7}{3}\right) A (k_B T)^{10/3} \text{Li}_{10/3}(z) \quad . \end{aligned}$$

¹Some sources use the notation $\zeta_q(z)$ for the polylogarithm, but for those of you who have yet to master the scribal complexities of the Greek ζ , you can use the notation $\text{Li}_q(z)$ instead.

(d) The Fermi energy is obtained from

$$n = \int_0^{\varepsilon_F} d\varepsilon g(\varepsilon) = \frac{A \varepsilon_F^{1+\sigma}}{1+\sigma} \quad \Rightarrow \quad \varepsilon_F(n) = \left(\frac{(1+\sigma)n}{A} \right)^{\frac{1}{1+\sigma}} = \left(\frac{7n}{3A} \right)^{3/7} .$$

We obtain the pressure from $p = -\left(\frac{\partial E}{\partial V}\right)_N$. The energy is

$$E = V \int_0^{\varepsilon_F} d\varepsilon g(\varepsilon) \varepsilon = V \cdot \frac{A \varepsilon_F^{2+\sigma}}{2+\sigma} \propto V^{-\frac{1}{1+\sigma}} .$$

Thus, $p = \frac{1}{1+\sigma} \cdot \frac{E}{V}$, i.e.

$$p(n) = \frac{A \varepsilon_F^{2+\sigma}}{(1+\sigma)(2+\sigma)} = \frac{3}{10} \left(\frac{7}{3}\right)^{3/7} A^{-3/7} n^{10/7} .$$

(5.4) At low energies, the conduction electron states in graphene can be described as fourfold degenerate fermions with dispersion $\varepsilon(\mathbf{k}) = \hbar v_F |\mathbf{k}|$. Graphene is a two-dimensional sheet of carbon. Using the Sommerfeld expansion,

- (a) Find the density of single particle states $g(\varepsilon)$.
- (b) Find the chemical potential $\mu(T, n)$ up to terms of order T^4 .
- (c) Find the energy density $\mathcal{E}(T, n) = E/V$ up to terms of order T^4 .

Solution :

(a) The DOS per unit volume is

$$g(\varepsilon) = 4 \int \frac{d^2k}{(2\pi)^2} \delta(\varepsilon - \hbar v_F k) = \frac{2\varepsilon}{\pi(\hbar v_F)^2} \quad .$$

(b) The Sommerfeld expansion is

$$\int_{-\infty}^{\infty} d\varepsilon f(\varepsilon - \mu) \phi(\varepsilon) = \int_{-\infty}^{\mu} d\varepsilon \phi(\varepsilon) + \frac{\pi^2}{6} (kT)^2 \phi'(\mu) + \frac{7\pi^4}{360} (k_B T)^4 \phi'''(\mu) + \dots \quad .$$

For the particle density, set $\phi(\varepsilon) = g(\varepsilon)$, in which case

$$n = \frac{1}{\pi} \left(\frac{\mu}{\hbar v_F} \right)^2 + \frac{\pi}{3} \left(\frac{k_B T}{\hbar v_F} \right)^2 \quad .$$

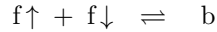
The expansion terminates after the $\mathcal{O}(T^2)$ term. Solving for μ ,

$$\begin{aligned} \mu(T, n) &= \hbar v_F (\pi n)^{1/2} \left[1 - \frac{\pi}{3n} \left(\frac{k_B T}{\hbar v_F} \right)^2 \right]^{1/2} \\ &= \hbar v_F (\pi n)^{1/2} \left\{ 1 - \frac{\pi}{6n} \left(\frac{k_B T}{\hbar v_F} \right)^2 - \frac{\pi^2}{72n^2} \left(\frac{k_B T}{\hbar v_F} \right)^4 + \dots \right\} \end{aligned}$$

(c) For the energy density \mathcal{E} , we take $\phi(\varepsilon) = \varepsilon g(\varepsilon)$, whence

$$\begin{aligned} \mathcal{E}(T, n) &= \frac{2\mu}{3\pi} \left[\left(\frac{\mu}{\hbar v_F} \right)^2 + \left(\frac{\pi k_B T}{\hbar v_F} \right)^2 \right] \\ &= \frac{2}{3} \sqrt{\pi} \hbar v_F n^{3/2} \left\{ 1 + \frac{\pi}{2n} \left(\frac{k_B T}{\hbar v_F} \right)^2 - \frac{\pi^2}{8n^2} \left(\frac{k_B T}{\hbar v_F} \right)^4 + \dots \right\} \end{aligned}$$

(5.5) Consider a system of N spin- $\frac{1}{2}$ particles occupying a volume V at temperature T . Opposite spin fermions may bind in a singlet state to form a boson:



with a binding energy $-\Delta < 0$. Assume that all the particles are nonrelativistic; the fermion mass is m and the boson mass is $2m$. Assume further that spin-flip processes exist, so that the \uparrow and \downarrow fermion species have identical chemical potential μ_f .

- (a) What is the equilibrium value of the boson chemical potential, μ_b ? *Hint*: the answer is $\mu_b = 2\mu_f$.
- (b) Let the total mass density be ρ . Derive the equation of state $\rho = \rho(\mu_f, T)$, assuming the bosons have not condensed. You may wish to abbreviate

$$\text{Li}_p(z) \equiv \sum_{n=1}^{\infty} \frac{z^n}{n^p} .$$

- (c) At what value of μ_f do the bosons condense?
- (d) Derive an equation for the Bose condensation temperature T_c . Solve this equation for T_c in the limits $\varepsilon_0 \ll \Delta$ and $\varepsilon_0 \gg \Delta$, respectively, where

$$\varepsilon_0 \equiv \frac{\pi\hbar^2}{m} \left(\frac{\rho/2m}{\zeta(\frac{3}{2})} \right)^{2/3} .$$

- (e) What is the equation for the condensate fraction $\rho_0(T, \rho)/\rho$ when $T < T_c$?

Solution :

(a) The chemical potential is the Gibbs free energy per particle. If the fermion and boson species are to coexist at the same T and p , the reaction $f\uparrow + f\downarrow \rightleftharpoons b$ must result in $\Delta G = \mu_b - 2\mu_f = 0$.

(b) For $T > T_c$,

$$\rho = -2m \lambda_T^{-3} \text{Li}_{3/2}(-e^{\mu_f/k_B T}) + 2\sqrt{8} m \lambda_T^{-3} \text{Li}_{3/2}(e^{(2\mu_f + \Delta)/k_B T}) ,$$

where $\lambda_T = \sqrt{2\pi\hbar^2/mk_B T}$ is the thermal wavelength for particles of mass m . This formula accounts for both fermion spin polarizations, each with number density $n_{f\uparrow} = n_{f\downarrow} = -\lambda_T^{-3} \text{Li}_{3/2}(-z_f)$ and the bosons with number density $\sqrt{8} \lambda_T^{-3} \text{Li}_{3/2}(z_b e^{\beta\Delta})$, with $z_b = z_f^2$ due to chemical equilibrium among the species. The factor of $2^{3/2} = \sqrt{8}$ arises from the fact that the boson mass is $2m$, hence the boson thermal wavelength is $\lambda_T/\sqrt{2}$.

(c) The bosons condense when $\mu_b = -\Delta$, the minimum single particle energy. This means $\mu_f = -\frac{1}{2}\Delta$. The equation of state for $T < T_c$ is then

$$\rho = -2m \lambda_T^{-3} \text{Li}_{3/2}(-e^{-\Delta/2k_B T}) + 4\sqrt{2} \zeta(\frac{3}{2}) m \lambda_T^{-3} + \rho_0 ,$$

where ρ_0 is the condensate mass density.

(d) At $T = T_c$ we have $\rho_0 = 0$, hence

$$\frac{\rho}{2m} \left(\frac{2\pi\hbar^2}{mk_B T_c} \right)^{3/2} = \sqrt{8} \zeta(\frac{3}{2}) - \text{Li}_{3/2}(-e^{-\Delta/2k_B T_c}) ,$$

which is a transcendental equation. Om. In the limit where Δ is very large, we have

$$T_c(\Delta \gg \varepsilon_0) = \frac{\pi\hbar^2}{mk_B} \left(\frac{\rho/2m}{\zeta(\frac{3}{2})} \right)^{2/3} = \frac{\varepsilon_0}{k_B} .$$

In the opposite limit, we have $\Delta \rightarrow 0^+$ and $-\text{Li}_{3/2}(-1) = \eta(3/2)$, where $\eta(s)$ is the Dirichlet η -function,

$$\eta(s) = \sum_{j=1}^{\infty} (-1)^{j-1} j^{-s} = (1 - 2^{1-s}) \zeta(s) \quad .$$

Then

$$T_c(\Delta \ll \varepsilon_0) = \frac{2\varepsilon_0/k_B}{(1 + \frac{3}{2}\sqrt{2})^{2/3}} \quad .$$

(e) The condensate fraction is

$$\nu = \frac{\rho_0}{\rho} = 1 - \left(\frac{T}{T_c}\right)^{3/2} \cdot \frac{\sqrt{8} \zeta(\frac{3}{2}) - \text{Li}_{3/2}(-e^{-\Delta/2k_B T})}{\sqrt{8} \zeta(\frac{3}{2}) - \text{Li}_{3/2}(-e^{-\Delta/2k_B T_c})} \quad .$$

Note that as $\Delta \rightarrow -\infty$ we have $-\text{Li}_{3/2}(-e^{-\Delta/2k_B T}) \rightarrow 0$ and the condensate fraction approaches the free boson result, $\nu = 1 - (T/T_c)^{3/2}$. In this limit there are no fermions present.

(5.6) A three-dimensional system of spin-0 bosonic particles obeys a dispersion relation $\varepsilon(\mathbf{k})$ with lowest energy $\varepsilon_0 = 0$. The Hamiltonian is given by

$$\hat{H} = \sum_{\mathbf{k}} \varepsilon(\mathbf{k}) \hat{n}_{\mathbf{k}} + \frac{U}{2V} \hat{N}^2 \quad ,$$

where $\hat{n}_{\mathbf{k}}$ is the number operator for particles with wavevector \mathbf{k} , $\hat{N} = \sum_{\mathbf{k}} \hat{n}_{\mathbf{k}}$ is the total number of particles, V is the volume of the system, and U is an interaction parameter with dimensions of $E \cdot L^3$.

(a) Treat the interaction term within mean field theory. That is, define $\hat{N} = \langle \hat{N} \rangle + \delta \hat{N}$, where $\langle \hat{N} \rangle$ is the thermodynamic average of \hat{N} , and derive the mean field self-consistency equation for the number density $n = \langle \hat{N} \rangle / V$ by neglecting terms quadratic in the fluctuations $\delta \hat{N}$. Show that the mean field Hamiltonian is

$$\hat{H}_{\text{MF}} = -\frac{1}{2} V U n^2 + \sum_{\mathbf{k}} [\varepsilon(\mathbf{k}) + U n] \hat{n}_{\mathbf{k}} \quad ,$$

(b) Derive the criterion for Bose condensation. Examine the cases $T < T_c(n)$ and $T > T_c(n)$. For $T > T_c(n)$, what is the relation between T , n , and μ ?

Solution :

(a) We write

$$\begin{aligned} \hat{N}^2 &= (\langle \hat{N} \rangle + \delta \hat{N})^2 \\ &= \langle \hat{N} \rangle^2 + 2 \langle \hat{N} \rangle \delta \hat{N} + (\delta \hat{N})^2 \\ &= -\langle \hat{N} \rangle^2 + 2 \langle \hat{N} \rangle \hat{N} + (\delta \hat{N})^2 \quad . \end{aligned}$$

We drop the last term, $(\delta \hat{N})^2$, because it is quadratic in the fluctuations. This is the mean field assumption. The

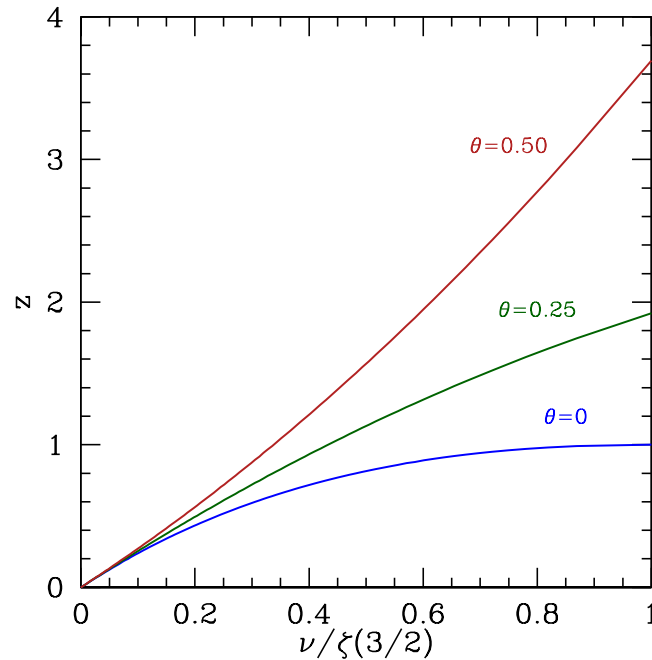


Figure 1: Fugacity z versus dimensionless density $\nu = n\lambda_T^3$.

Hamiltonian now becomes

$$\mathcal{H}_{\text{MF}} = -\frac{1}{2}VUn^2 + \sum_{\mathbf{k}} [\varepsilon(\mathbf{k}) + Un] \hat{n}_{\mathbf{k}} \quad ,$$

where $n = \langle \hat{N} \rangle / V$ is the number density. This, the dispersion is effectively changed, to

$$\tilde{\varepsilon}(\mathbf{k}) = \frac{\hbar^2 \mathbf{k}^2}{2m} + Un \quad .$$

The average number of particles in state $|\mathbf{k}\rangle$ is given by the Bose function,

$$\langle \hat{n}_{\mathbf{k}} \rangle = \frac{1}{\exp[\tilde{\varepsilon}(\mathbf{k})/k_{\text{B}}T] - 1} \quad .$$

(b) At criticality, we must have $\mu = \min_{\mathbf{k}} \tilde{\varepsilon}(\mathbf{k}) = Un$, and the critical number density $n_{\text{c}}(T)$ is given by

$$n_{\text{c}}(T) = \int_0^{\infty} d\varepsilon \frac{g(\varepsilon)}{e^{\varepsilon/k_{\text{B}}T} - 1} \quad ,$$

which may be inverted to yield $T_{\text{c}}(n)$.

$$T < T_{\text{c}}(n) \quad : \quad n(T, n_0) = n_0 + n_{\text{c}}(T) \quad (n_0 > 0, \mu = Un)$$

$$T > T_{\text{c}}(n) \quad : \quad n(T, \mu) = n_{\text{c}}(T) = \int_0^{\infty} d\varepsilon \frac{g(\varepsilon)}{e^{(\varepsilon+Un-\mu)/k_{\text{B}}T} - 1} \quad (n_0 = 0, \mu < Un) \quad ,$$

For ballistic particles we define $\nu \equiv n\lambda_T^3$, where $\lambda_T = \sqrt{2\pi\hbar^2/mk_{\text{B}}T}$ is the thermal wavelength. We then have for $T > T_{\text{c}}(n)$

$$\nu = \text{Li}_{3/2}(z e^{-\theta\nu})$$

with $\theta \equiv U/k_{\text{B}}T\lambda_T^3 \propto UT^{1/2}$ a dimensionless parameter formed from U and T . This may be considered an equation of state relating the three intensive quantities (θ, z, ν) , or, equivalently, (T, μ, n) . In Fig. 1 we show $z(\nu)$ for three different values of θ .

(5.7) A three-dimensional gas of particles obeys the dispersion $\varepsilon(\mathbf{k}) = A k^{5/2}$. There are no internal degrees of freedom (*i.e.* the degeneracy factor is $g = 1$). The number density is n .²

- (a) Compute the single particle density of states $g(\varepsilon)$.
- (b) For bosons, compute the condensation temperature $T_{\text{BEC}}(n)$.
- (c) For fermions, compute the ground state energy density $e_0(n)$.
- (d) For photon statistics, compute the temperature $T(n)$.
- (e) For photon statistics, compute the entropy density $s(n) = S/V$.
- (f) For bosons and fermions, compute the second virial coefficient $B_2(T)$.

Solution :

(a) With $\varepsilon = A k^\sigma$ we have $k(\varepsilon) = (\varepsilon/A)^{1/\sigma}$, and

$$g(\varepsilon) = \frac{1}{2\pi^2} \frac{k^2}{\varepsilon'(k)} \Big|_{k=k(\varepsilon)} = \frac{\varepsilon^{\frac{3}{\sigma}-1}}{2\pi^2 \sigma A^{3/\sigma}} = \frac{\varepsilon^{1/5}}{5\pi^2 A^{6/5}} .$$

(b) The number density $n(T, z, n_0)$ for bosons, in the grand canonical ensemble, is

$$n(T, z, n_0) = \int_0^\infty d\varepsilon \frac{g(\varepsilon)}{z^{-1} e^{\varepsilon/k_B T} - 1} + n_0 ,$$

where n_0 is the condensate density. For $T < T_{\text{BEC}}$, we have $z = 1$ and $n_0 > 0$. For $T > T_{\text{BEC}}$, we have $z < 1$ and $n_0 = 0$. Precisely at $T = T_{\text{BEC}}$, both conditions apply: $z = 1$ and $n_0 = 0$. Thus,

$$n = \int_0^\infty d\varepsilon \frac{g(\varepsilon)}{e^{\varepsilon/k_B T_c} - 1} = \frac{\Gamma(\frac{3}{\sigma}) \zeta(\frac{3}{\sigma})}{2\pi^2 \sigma} \left(\frac{k_B T_c}{A} \right)^{3/\sigma} = \frac{\Gamma(\frac{6}{5}) \zeta(\frac{6}{5})}{5\pi^2} \left(\frac{k_B T_c}{A} \right)^{6/5} .$$

Thus,

$$T_{\text{BEC}}(n) = \left(\frac{2\pi^2 \sigma n}{\Gamma(\frac{3}{\sigma}) \zeta(\frac{3}{\sigma})} \right)^{\sigma/3} \cdot \frac{A}{k_B} = \left(\frac{5\pi^2 n}{\Gamma(\frac{6}{5}) \zeta(\frac{6}{5})} \right)^{5/6} \cdot \frac{A}{k_B} .$$

(c) The ground state energy density for spinless (*i.e.* $g = 1$) fermions is

$$\varepsilon_0 = \frac{E_0}{V} = \int \frac{d^3k}{(2\pi)^3} A k^\sigma \Theta(k_F - k) = \frac{A}{2\pi^2} \frac{k_F^{3+\sigma}}{3+\sigma} .$$

The number density is

$$n = \frac{N}{V} = \int \frac{d^3k}{(2\pi)^3} \Theta(k_F - k) = \frac{k_F^3}{6\pi^2} \implies k_F = (6\pi^2 n)^{1/3} .$$

Thus,

$$\varepsilon_0(n) = \frac{(6\pi^2)^{\sigma/3}}{1 + \frac{\sigma}{3}} \cdot A n^{1+\frac{\sigma}{3}} = \frac{6}{11} (6\pi^2)^{5/6} \cdot A n^{11/6} .$$

²We will solve the problem for the more general dispersion $\varepsilon(k) = A k^\sigma$ and then indicate the result for $\sigma = \frac{5}{2}$.

(d) The photon density is

$$n = \int_0^{\infty} d\varepsilon \frac{g(\varepsilon)}{e^{\varepsilon/k_B T} - 1} ,$$

which is the same expression as in part (b) above! Thus,

$$T(n) = \left(\frac{2\pi^2 \sigma n}{\Gamma(\frac{3}{\sigma}) \zeta(\frac{3}{\sigma})} \right)^{\sigma/3} \frac{A}{k_B} = \left(\frac{5\pi^2 n}{\Gamma(\frac{6}{5}) \zeta(\frac{6}{5})} \right)^{5/6} \frac{A}{k_B} .$$

(e) The grand potential is

$$\Omega(T, V) = V k_B T \int_0^{\infty} d\varepsilon g(\varepsilon) \ln(1 - e^{-\varepsilon/k_B T}) = -V \int_0^{\infty} d\varepsilon \frac{H(\varepsilon)}{e^{\varepsilon/k_B T} - 1} ,$$

where $g(\varepsilon) = H'(\varepsilon)$. Integrating $g(\varepsilon)$ to obtain $H(\varepsilon)$, we have

$$\Omega(T, V) = -\frac{V}{6\pi^2 A^{3/\sigma}} \int_0^{\infty} d\varepsilon \frac{\varepsilon^{3/\sigma}}{e^{\varepsilon/k_B T} - 1} = -\frac{\Gamma(\frac{3}{\sigma} + 1) \zeta(\frac{3}{\sigma})}{6\pi^2 A^{3/\sigma}} V (k_B T)^{1+\frac{3}{\sigma}}$$

The entropy density is then

$$s(T) = -\frac{1}{V} \frac{\partial \Omega}{\partial T} = \frac{\Gamma(\frac{3}{\sigma} + 2) \zeta(\frac{3}{\sigma} + 1)}{6\pi^2} \left(\frac{k_B T}{A} \right)^{3/\sigma} k_B ,$$

The number density, as we have seen, is

$$n(T) = \frac{\Gamma(\frac{3}{\sigma}) \zeta(\frac{3}{\sigma})}{2\pi^2 \sigma} \left(\frac{k_B T}{A} \right)^{3/\sigma} ,$$

hence

$$s(n) = \frac{\zeta(\frac{3}{\sigma} + 1)}{\zeta(\frac{3}{\sigma})} \cdot (\frac{3}{\sigma} + 1) n k_B = \frac{\zeta(\frac{11}{5})}{\zeta(\frac{6}{5})} \cdot \frac{11}{5} n k_B .$$

On dimensionful grounds, we knew *a priori* that $s(n) \propto n k_B$.

(f) We have

$$n = \int_0^{\infty} d\varepsilon \frac{g(\varepsilon)}{z^{-1} e^{\varepsilon/k_B T} - 1} = \pm \frac{\Gamma(\frac{3}{\sigma})}{2\pi^2 \sigma} \left(\frac{k_B T}{A} \right)^{3/\sigma} \text{Li}_{\frac{3}{\sigma}}(\pm z)$$

$$\frac{p}{k_B T} = \int_0^{\infty} d\varepsilon \frac{H(\varepsilon)}{z^{-1} e^{\varepsilon/k_B T} - 1} = \pm \frac{\Gamma(\frac{3}{\sigma})}{2\pi^2 \sigma} \left(\frac{k_B T}{A} \right)^{3/\sigma} \text{Li}_{\frac{3}{\sigma}+1}(\pm z) ,$$

where the top sign is for bosons and the bottom for fermions. It helps to define the thermal wavelength

$$\lambda_T \equiv \left(\frac{2\pi^2 \sigma}{\Gamma(\frac{3}{\sigma})} \right)^{1/3} \cdot \left(\frac{k_B T}{A} \right)^{1/\sigma} = \left(\frac{5\pi^2}{\Gamma(\frac{6}{5})} \right)^{1/3} \left(\frac{A}{k_B T} \right)^{2/5} ,$$

so

$$n \lambda_T^3 = \pm \text{Li}_{\frac{3}{\sigma}}(\pm z) = z \pm 2^{-3/\sigma} z^2 + \mathcal{O}(z^3)$$

$$\frac{p \lambda_T^3}{k_B T} = \pm \text{Li}_{\frac{3}{\sigma}+1}(\pm z) = z \pm 2^{-1-(3/\sigma)} z^2 + \mathcal{O}(z^3) .$$

From the first of these, we have

$$z = n\lambda_T^3 \mp 2^{-3/\sigma} n^2 \lambda_T^6 + \mathcal{O}(n^3 \lambda_T^9) \quad .$$

Substituting this into the second equation, we obtain the lowest nontrivial term in the virial expansion of the equation of state:

$$\frac{p}{k_B T} = n \mp 2^{-1-(3/\sigma)} n^2 \lambda_T^3 + \mathcal{O}(n^3 \lambda_T^6) \quad .$$

The second virial coefficient is then

$$B_2(T) = \mp 2^{-1-(3/\sigma)} \lambda_T^3 = \mp \frac{5\pi^2}{2^{11/5} \Gamma(\frac{6}{5})} \left(\frac{A}{k_B T} \right)^{6/5} \quad .$$

(5.8) Consider a three-dimensional gas of noninteracting quantum particles with dispersion $\varepsilon(\mathbf{k}) = A |\mathbf{k}|^{3/2}$.

- Find the single particle density of states per unit volume $g(\varepsilon)$.
- Find expressions for $n(T, z)$ and $p(T, z)$, each expressed as power series in the fugacity z , for both Bose-Einstein and Fermi-Dirac statistics.
- Find the virial expansion for the equation of state up to terms of order n^3 , for both bosons and fermions.

Solution :

(a) The density of states for dispersion $\varepsilon(\mathbf{k}) = A |\mathbf{k}|^\sigma$ is

$$\begin{aligned} g(\varepsilon) &= \mathbf{g} \int \frac{d^d k}{(2\pi)^d} \delta(\varepsilon - A k^\sigma) \\ &= \frac{\mathbf{g} \Omega_d}{(2\pi)^d} \int_0^\infty dk k^{d-1} \frac{\delta(k - (\varepsilon/A)^{1/\sigma})}{\sigma A k^{\sigma-1}} = D \varepsilon^{\frac{d}{\sigma}-1} \quad , \end{aligned}$$

with

$$D = \frac{2\mathbf{g}}{(2\sqrt{\pi})^d \sigma \Gamma(d/2)} A^{-d/\sigma} \quad .$$

(b) We have

$$\begin{aligned} n(T, z) &= \sum_{j=1}^{\infty} (\pm 1)^{j-1} C_j(T) z^j \\ p(T, z) &= k_B T \sum_{j=1}^{\infty} (\pm 1)^{j-1} z^j j^{-1} C_j(T) z^j \quad , \end{aligned}$$

where

$$C_j(T) = \int_0^\infty d\varepsilon g(\varepsilon) e^{-j\varepsilon/k_B T} = D \Gamma(d/\sigma) \left(\frac{k_B T}{j} \right)^{d/\sigma} \quad .$$

Thus, we have

$$\begin{aligned} \pm n v_T &= \sum_{j=1}^{\infty} j^{-r} (\pm z)^j \\ \pm p v_T / k_B T &= \sum_{j=1}^{\infty} j^{-(r+1)} (\pm z)^j \quad , \end{aligned}$$

where $r = d/\sigma$ and

$$v_T = \frac{1}{D \Gamma(d/\sigma) (k_B T)^{d/\sigma}} = \frac{(2\sqrt{\pi})^d \sigma \Gamma(d/2)}{2\mathbf{g} D \Gamma(d/\sigma)} \left(\frac{A}{k_B T} \right)^{d/\sigma} \quad .$$

has dimensions of volume.

(c) We now let $x = \pm z$, and interrogate Mathematica:

```
In[1]= y = InverseSeries[x + x^2/2^r + x^3/3^r + x^4/4^r + O[x]^5]
```

```
In[2]= w = y + y^2/2^(r+1) + y^3/3^(r+1) + y^4/4^(r+1) + O[y]^5 .
```

The result is

$$p = nk_{\text{B}}T \left[1 + B_2(T)n + B_3(T)n^2 + \dots \right] ,$$

where

$$B_2(T) = \mp 2^{-(r+1)} v_T$$

$$B_3(T) = \left(2^{-2r} - 2 \cdot 3^{-(r+1)} \right) v_T^2$$

$$B_4(T) = \pm 2^{-(3r+1)} 3^{1-r} \left(2^{2r+1} - 5 \cdot 3^{r-1} - 2^{r-1} 3^r \right) v_T^3 .$$

Substitute $\sigma = \frac{3}{2}$ to find the solution for the conditions given.

(5.9) You know that at most one fermion may occupy any given single-particle state. A *parafermion* is a particle for which the maximum occupancy of any given single-particle state is k , where k is an integer greater than zero. (For $k = 1$, parafermions are regular everyday fermions; for $k = \infty$, parafermions are regular everyday bosons.) Consider a system with one single-particle level whose energy is ε , i.e. the Hamiltonian is simply $\mathcal{H} = \varepsilon n$, where n is the particle number.

- (a) Compute the partition function $\Xi(\mu, T)$ in the grand canonical ensemble for parafermions.
- (b) Compute the occupation function $n(\mu, T)$. What is n when $\mu = -\infty$? When $\mu = \varepsilon$? When $\mu = +\infty$? Does this make sense? Show that $n(\mu, T)$ reduces to the Fermi and Bose distributions in the appropriate limits.
- (c) Sketch $n(\mu, T)$ as a function of μ for both $T = 0$ and $T > 0$.

Solution:

The general expression for Ξ is

$$\Xi = \prod_{\alpha} \sum_{n_{\alpha}} (z e^{-\beta \varepsilon_{\alpha}})^{n_{\alpha}} .$$

Now the sum on n runs from 0 to k , and

$$\sum_{n=0}^k x^n = \frac{1 - x^{k+1}}{1 - x} .$$

(a) Thus,

$$\Xi = \frac{1 - e^{(k+1)\beta(\mu-\varepsilon)}}{1 - e^{\beta(\mu-\varepsilon)}} .$$

(b) We then have

$$\begin{aligned} n &= -\frac{\partial \Omega}{\partial \mu} = \frac{1}{\beta} \frac{\partial \ln \Xi}{\partial \mu} \\ &= \frac{1}{e^{\beta(\varepsilon-\mu)} - 1} - \frac{k+1}{e^{(k+1)\beta(\varepsilon-\mu)} - 1} \end{aligned}$$

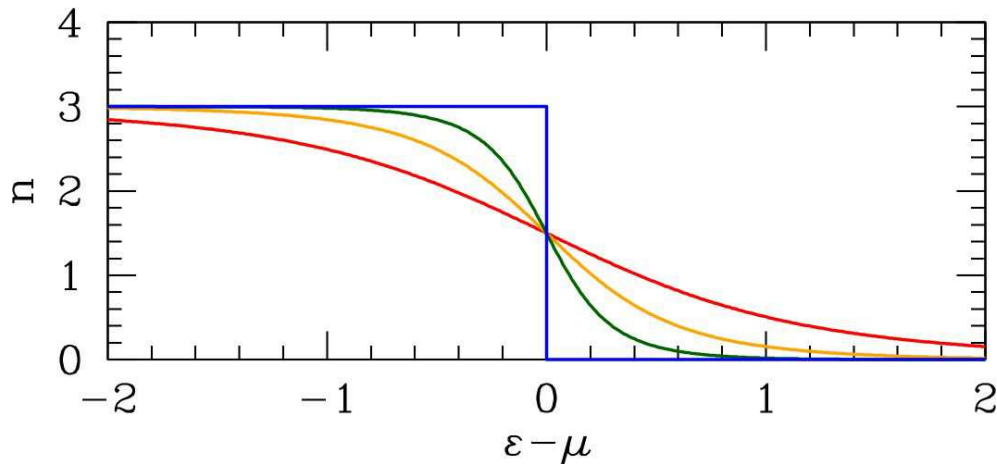


Figure 2: labelpara $k = 3$ parafermion occupation number *versus* $\varepsilon - \mu$ for $k_B T = 0$, $k_B T = 0.25$, $k_B T = 0.5$, and $k_B T = 1$.

- (c) A plot of $n(\varepsilon, T, \mu)$ for $k = 3$ is shown in Fig. ?? . Qualitatively the shape is that of the Fermi function $f(\varepsilon - \mu)$. At $T = 0$, the occupation function is $n(\varepsilon, T = 0, \mu) = k \Theta(\mu - \varepsilon)$. This step function smooths out for T finite.
- (d) For each $k < \infty$, the occupation number $n(z, T)$ is a finite order polynomial in z , and hence an analytic function of z . Therefore, there is no possibility for Bose condensation except for $k = \infty$.

(5.10) A gas of quantum particles with photon statistics has dispersion $\varepsilon(\mathbf{k}) = A |\mathbf{k}|^4$.

- (a) Find the single particle density of states per unit volume $g(\varepsilon)$.
- (b) Repeat the arguments in ch. 5 of the lecture notes for this dispersion.
- (c) Assuming our known values for the surface temperature of the sun, the radius of the earth-sun orbit, and the radius of the earth, what would you expect the surface temperature of the earth to be if the sun radiated particles with this dispersion instead of photons?

Solution :

(a) See the solution to part (a) of problem 8 above. For $d = 3$ and $\sigma = 4$ we have

$$g(\varepsilon) = \frac{\mathfrak{g}}{2\pi^2} A^{-3/4} \varepsilon^{-1/4} .$$

(b) Scaling volume by λ scales the lengths by $\lambda^{1/3}$, the quantized wavevectors by $\lambda^{-1/3}$, and the energy eigenvalues by $\lambda^{-4/3}$, since $\varepsilon \propto k^4$. Thus,

$$p = - \left(\frac{\partial E}{\partial V} \right)_S = \frac{4E}{3V} ,$$

which says

$$\left(\frac{\partial E}{\partial V} \right)_T = T \left(\frac{\partial p}{\partial T} \right)_V - p = \frac{3}{4} p \Rightarrow p(T) = BT^{7/4} .$$

Indeed,

$$\begin{aligned} p(T) &= -k_B T \int_{-\infty}^{\infty} g(\varepsilon) \ln(1 - e^{-\varepsilon/k_B T}) \\ &= -\frac{\mathfrak{g}}{2\pi^2} A^{3/4} (k_B T)^{7/4} \int_{-\infty}^{\infty} du u^{-1/4} \ln(1 - e^{-u}) . \end{aligned}$$

(c) See ch. 5 of the lecture notes. Assume a dispersion of the form $\varepsilon(k)$ for the (nonconserved) bosons. Then the energy current incident on a differential area dA of surface normal to \hat{z} is

$$dP = dA \cdot \int \frac{d^3k}{(2\pi)^3} \Theta(\cos\theta) \cdot \varepsilon(k) \cdot \frac{1}{\hbar} \frac{\partial \varepsilon(k)}{\partial k_z} \cdot \frac{1}{e^{\varepsilon(k)/k_B T} - 1} .$$

Note that

$$\frac{\partial \varepsilon(k)}{\partial k_z} = \frac{k_z}{k} \frac{\partial \varepsilon}{\partial k} = \cos\theta \varepsilon'(k) .$$

Now let us assume a power law dispersion $\varepsilon(k) = Ak^\alpha$. Changing variables to $t = Ak^\alpha/k_B T$, we find

$$\frac{dP}{dA} = \sigma T^{2+\frac{2}{\alpha}} ,$$

where

$$\sigma = \zeta\left(2 + \frac{2}{\alpha}\right) \Gamma\left(2 + \frac{2}{\alpha}\right) \cdot \frac{\mathfrak{g} k_B^{2+\frac{2}{\alpha}} A^{-\frac{2}{\alpha}}}{8\pi^2 \hbar} .$$

One can check that for $g = 2$, $A = \hbar c$, and $\alpha = 1$ that this result reduces to Stefan's Law. Equating the power

incident on the earth to that radiated by the earth,

$$4\pi R_{\odot}^2 \cdot \sigma T_{\odot}^{2(1+\alpha^{-1})} \cdot \frac{\pi R_e^2}{4\pi a_e^2} = 4\pi R_e^2 \cdot \sigma T_e^{2(1+\alpha^{-1})} \quad ,$$

which yields

$$T_e = \left(\frac{R_{\odot}}{2a_e} \right)^{\frac{\alpha}{\alpha+1}} T_{\odot} \quad .$$

Plugging in the appropriate constants and setting $\alpha = 4$, we obtain $T_e = 45.2$ K. Brrr!

(5.11) Consider a three-dimensional ultrarelativistic gas, with dispersion $\varepsilon = \hbar c|\mathbf{k}|$. Find the virial expansion of the equation of state $p = p(n, T)$ to order n^3 for both bosons and fermions.

Solution : We have

$$\beta p = \mp g \int \frac{d^3k}{(2\pi)^3} \ln(1 \mp z e^{-\beta\varepsilon(\mathbf{k})})$$

$$z = g \int \frac{d^3k}{(2\pi)^3} \frac{1}{z^{-1} e^{\beta\varepsilon(\mathbf{k})} \mp 1} ,$$

where g is the degeneracy of each \mathbf{k} mode. With $\varepsilon(\mathbf{k}) = \hbar ck$, we change variables to $t = \beta\hbar ck$ and find

$$\beta p = \frac{g}{6\pi^2} \left(\frac{k_B T}{\hbar c}\right)^3 \int_{-\infty}^{\infty} dt \frac{t^3}{z^{-1} e^t \mp 1} = \frac{g}{\pi^2} \left(\frac{k_B T}{\hbar c}\right)^3 \sum_{j=1}^{\infty} (\pm 1)^{j-1} \frac{z^j}{j^4}$$

$$n = \frac{g}{2\pi^2} \left(\frac{k_B T}{\hbar c}\right)^3 \int_{-\infty}^{\infty} dt \frac{t^2}{z^{-1} e^t \mp 1} = \frac{g}{\pi^2} \left(\frac{k_B T}{\hbar c}\right)^3 \sum_{j=1}^{\infty} (\pm 1)^{j-1} \frac{z^j}{j^3} ,$$

where we have integrated by parts in the first of these equations. Now it's time to ask Mathematica :

In[1] = y = InverseSeries[x + x^2/2^3 + x^3/3^3 + x^4/4^3 + x^5/5^3 + O[x]^6]

Out[1] = x - $\frac{x^2}{8}$ - $\frac{5x^3}{864}$ - $\frac{31x^4}{13824}$ - $\frac{56039x^5}{62208000}$ + O[x]^6

In[2] = w = y + y^2/2^4 + y^3/3^4 + y^4/4^4 + y^5/5^4

Out[2] = x - $\frac{x^2}{16}$ - $\frac{47x^3}{5184}$ - $\frac{25x^4}{9216}$ - $\frac{2014561x^5}{1866240000}$ + O[x]^6

So with the definition

$$\lambda_T = \pi^{2/3} g^{-1/3} \frac{\hbar c}{k_B T} ,$$

we have

$$p = nk_B T (1 + B_2 n + B_3 n^2 + \dots) ,$$

where

$$B_2 = \mp \frac{1}{16} \lambda_T^3 , \quad B_3 = -\frac{47}{5184} \lambda_T^6 , \quad B_4 = \mp \frac{25}{9216} \lambda_T^9 , \quad B_5 = -\frac{2014561}{1866240000} \lambda_T^{12} .$$

(5.11) Almost all elements freeze into solids well before they can undergo Bose condensation. Setting the Lindemann temperature equal to the Bose condensation temperature, show that this implies a specific ratio of $k_B \Theta_D$ to \hbar^2/Ma^2 , where M is the atomic mass and a is the lattice spacing. Evaluate this ratio for the noble gases He, Ne, Ar, Kr, and Xe. (You will have to look up some numbers.)

Solution : The Lindemann melting temperature T_M and the Bose condensation temperature T_c for monatomic solids are given by

$$T_M = x^2 \cdot \frac{M k_B \Theta_D^2 a^2}{9 \hbar^2} \quad , \quad T_c = \frac{2\pi \hbar^2}{M k_B} \left(\frac{n}{\zeta(3/2)} \right)^{2/3} \quad ,$$

where a is the lattice constant, M the atomic mass, and Θ_D the Debye temperature. For a simple cubic lattice, the number density is $n = a^{-3}$. Helium solidifies into a hexagonal close packed (HCP) structure, while Neon, Argon, Krypton, and Xenon solidify into a face-centered cubic (FCC) structure. The unit cell volume for both HCP and FCC is $a^3/\sqrt{2}$, where a is the lattice spacing, so $n = \sqrt{2} a^{-3}$ for the rare gas solids. Thus, we find

$$\frac{T_M}{T_c} = \frac{x}{\alpha} \cdot \left(\frac{k_B \Theta_D}{\hbar^2/Ma^2} \right)^2 \quad .$$

where

$$\alpha = 18\pi \left(\frac{\sqrt{2}}{\zeta(3/2)} \right)^{2/3} \approx 40 \quad .$$

If we set $x = 0.1$ we find $\frac{x}{\alpha} \approx \frac{1}{400}$. Now we need some data for Θ_D and a . The most convenient table of data I've found is from H. Glyde's article on solid helium in the *Encyclopedia of Physics*. The table entry for ^4He is for the BCC structure at a pressure $p = 25$ bar. For a BCC structure the unit cell volume is $4a^3/3\sqrt{3}$. Define the ratio $R \equiv k_B \Theta_D / (\hbar^2/Ma^2)$.

As one can see from Tab. 1 and from the above equation for T_M/T_c , the R values are such that the melting temperature is predicted to be several orders of magnitude higher than the ideal Bose condensation temperature in every case except ^4He , where the ratio is on the order of unity (and is less than unity if the actual melting temperature is used). The reason that ^4He under high pressure is a solid rather than a Bose condensate at low temperatures is because the ^4He atoms are not free particles.

crystal	a (Å)	M (amu)	Θ_D (K)	T_M^{actual} (K)	T_c	$\hbar^2/Ma^2 k_B$ (K)	R
^4He	3.57	4.00	25	1.6	3.9	0.985	25
Ne	4.46	20.2	66	24.6	0.50	0.125	530
Ar	5.31	39.9	84	83.8	0.18	0.0446	1900
Kr	5.65	83.8	64	161.4	0.076	0.0188	3400
Xe	6.13	131	55	202.0	0.041	0.0102	20000

Table 1: Lattice constants for Ne, Ar, Kr, and Xe from F. W. de Wette and R. M. J. Cotterill, *Solid State Comm.* **6**, 227 (1968). Debye temperatures and melting temperatures from H. Glyde, *Solid Helium* in *Encyclopedia of Physics*. ^4He data are for $p = 25$ bar, in the bcc phase (from Glyde).

(5.13) A nonrelativistic Bose gas consists of particles of spin $S = 1$. Each boson has mass m and magnetic moment μ_0 . A gas of these particles is placed in an external field H .

(a) What is the relationship of the Bose condensation temperature $T_c(H)$ to $T_c(H = 0)$ when $\mu_0 H \gg k_B T$?

(b) Find the magnetization M for $T < T_c$ when $\mu_0 H \gg k_B T$. Calculate through order $\exp(-\mu_0 H/k_B T)$.

Solution :

The number density of bosons is given by

$$n(T, z) = \lambda_T^{-3} \left\{ \text{Li}_{3/2}(z e^{\mu_0 H/k_B T}) + \text{Li}_{3/2}(z) + \text{Li}_{3/2}(z e^{-\mu_0 H/k_B T}) \right\} .$$

The argument of $\text{Li}_s(z)$ cannot exceed unity, thus Bose condensation occurs for $z = \exp(-\mu_0 H/k_B T)$ (assuming $H > 0$). Thus, the condition for Bose condensation is given by

$$n \lambda_{T_c}^3 = \zeta(3/2) + \text{Li}_{3/2}(e^{-\mu_0 H/k_B T_c}) + \text{Li}_{3/2}(e^{-2\mu_0 H/k_B T_c}) .$$

This is a transcendental equation for $T = T_c(n, H)$. In the limit $\mu_0 H \gg k_B T_c$, the second two terms become negligible, since

$$\text{Li}_s(z) = \sum_{j=1}^{\infty} \frac{z^j}{j^s} .$$

Thus,

$$T_c(H \rightarrow \infty) = \frac{2\pi\hbar^2}{m} \left(\frac{n}{\zeta(3/2)} \right)^{2/3} .$$

When $H = 0$, we have Thus,

$$T_c(H \rightarrow 0) = \frac{2\pi\hbar^2}{m} \left(\frac{n}{3\zeta(3/2)} \right)^{2/3} .$$

Thus,

$$\frac{T_c(H \rightarrow \infty)}{T_c(H \rightarrow 0)} = 3^{2/3} = 2.08008 \dots$$

The magnetization density is

$$M = \mu_0 \lambda_T^{-3} \left\{ \text{Li}_{3/2}(z e^{\mu_0 H/k_B T}) - \text{Li}_{3/2}(z e^{-\mu_0 H/k_B T}) \right\} .$$

For $T < T_c$, we have $z = \exp(-\mu_0 H/k_B T)$ and therefore

$$\begin{aligned} M &= \mu_0 \lambda_T^{-3} \left\{ \zeta(3/2) - \sum_{j=1}^{\infty} j^{-3/2} e^{-2j\mu_0 H/k_B T} \right\} \\ &= n \mu_0 \left\{ 1 - \frac{e^{-2\mu_0 H/k_B T}}{\zeta(3/2)} + \mathcal{O}(e^{-4\mu_0 H/k_B T}) \right\} \end{aligned}$$

(5.14) Consider a set of N noninteracting $S = \frac{1}{2}$ fermions in a one-dimensional harmonic oscillator potential. The oscillator frequency is ω . For $k_B T \ll \hbar\omega$, find the lowest order nontrivial contribution to the heat capacity $C(T)$, using the ordinary canonical ensemble. The calculation depends on whether N is even or odd, so be careful! Then repeat your calculation for $S = \frac{3}{2}$.

Solution :

The partition function is given by

$$Z = g_0 e^{-\beta E_0} + g_1 e^{-\beta E_1} + \dots ,$$

where g_j and E_j are the degeneracy and energy of the j^{th} energy level, respectively. From this, we have

$$F = -k_B T \ln Z = E_0 - k_B T \ln(g_0 + g_1 e^{-\Delta_1/k_B T} + \dots) ,$$

where $\Delta_j \equiv E_j - E_0$ is the excitation energy for energy level $j > 0$. Suppose that the spacings between consecutive energy levels are much larger than the temperature, i.e. $E_{j+1} - E_j \gg k_B T$. This is the case for any harmonic oscillator system so long as $\hbar\omega \gg k_B T$, where ω is the oscillator frequency. We then have

$$F = E_0 - k_B T \ln g_0 - \frac{g_1}{g_0} k_B T e^{-\Delta_1/k_B T} + \dots$$

The entropy is

$$S = -\frac{\partial F}{\partial T} = \ln g_0 + \frac{g_1}{g_0} e^{-\Delta_1/k_B T} + \frac{g_1}{g_0} \frac{\Delta_1}{T} e^{-\Delta_1/k_B T} + \dots$$

and thus the heat capacity is

$$C(T) = T \frac{\partial S}{\partial T} = \frac{g_1}{g_0} \frac{\Delta_1^2}{k_B T^2} e^{-\Delta_1/k_B T} + \dots$$

With $g_0 = g_1 = 1$, this recovers what we found in ch. 4 of the lecture notes for the low temperature behavior of the Schottky two level system.

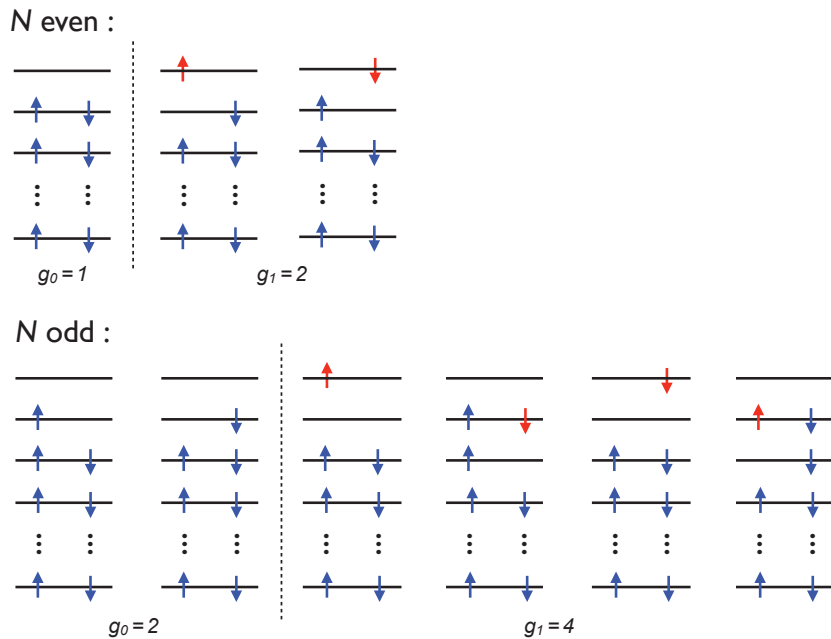


Figure 3: Ground states and first excited states for the $S = \frac{1}{2}$ one-dimensional simple harmonic oscillator.

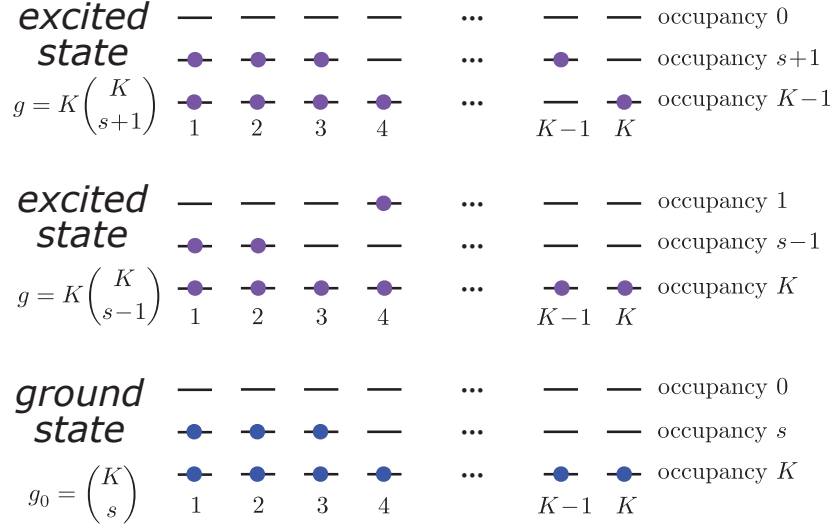


Figure 4: Ground states and first excited states for the general S case, with $K = 2S + 1$.

OK, so now let us consider the problem at hand, which is the one-dimensional harmonic oscillator, whose energy levels lie at $E_j = (j + \frac{1}{2})\hbar\omega$, hence $\Delta_j = j\hbar\omega$ is the j^{th} excitation energy. For $S = \frac{1}{2}$, each level is twofold degenerate. When N is even, the ground state is unique, and we occupy states $|j, \uparrow\rangle$ and $|j, \downarrow\rangle$ for $j \in \{0, \dots, \frac{N}{2} - 1\}$. Thus, the ground state is nondegenerate and $g_0 = 1$. The lowest energy excited states are then made, at fixed total particle number N , by promoting either of the $|j = \frac{N}{2} - 1, \sigma\rangle$ levels ($\sigma = \uparrow$ or \downarrow) to $j = \frac{N}{2}$. There are $g_1 = 2$ ways to do this, each of which increases the energy by $\Delta_1 = \hbar\omega$. When N is odd, we fill one of the two spin species up to level $j = \frac{N-1}{2}$ and the other up to level $j = \frac{N+1}{2}$. In this case $g_0 = 2$. What about the excited states? It turns out that $g_1 = 4$, as can be seen from the diagrams in Fig. 3. For N odd, in either of the two ground states, the highest occupied oscillator level is $j = \frac{N+1}{2}$, which is only half-occupied with one of the two spin species. To make an excited state, one can either (i) promote the occupied state to the next oscillator level $j = \frac{N+3}{2}$, or (ii) fill the unoccupied state by promoting the occupied state from the $j = \frac{N-1}{2}$ level. So $g_1 = 2 \cdot 2 = 4$. Thus, for either possibility regarding the parity of N , we have $g_1/g_0 = 2$, which means

$$C(T) = \frac{2(\hbar\omega)^2}{k_B T^2} e^{-\hbar\omega/k_B T} + \dots$$

This result is valid for $N > 1$.

An exception occurs when $N = 1$, where the lone particle is in the $n = 0$ oscillator level. Since there is no $n = -1$ level, the excited state degeneracy is then $g_1 = 2$, and the heat capacity is half the above value. Of course, for $N = 0$ we have $C = 0$.

What happens for general spin S ? Now each oscillator level has a $K \equiv 2S + 1$ spin degeneracy. We may write $N = rK + s$, where r and s are integers and $s \in \{0, 1, \dots, K-1\}$. The ground states are formed by fully occupying all $|j, m\rangle$ states, with $m \in \{1, \dots, K\}$, from $j = 0$ to $j = r-1$. The remaining s particles must all be placed in the K degenerate levels at $j = r$, and there are $\binom{K}{s}$ ways of achieving this. Thus, $g_0 = \binom{K}{s}$.

Now consider the excited states. We first assume $r > 0$. There are then two ways to make an excited state. If $s > 0$, we can promote one of the s occupied states with $j = r$ to the next oscillator level $j = r+1$. One then has $s-1$ of the K states with $j = r$ occupied, and one of the K states with $j = r+1$ occupied. The degeneracy for this configuration is $g = \binom{K}{1} \binom{K}{s-1} = K \binom{K}{s-1}$. Another possibility is to promote one of the filled $j = r-1$ levels to the $j = r$ level, resulting in $K-1$ occupied states with $j = r-1$ and $s+1$ occupied states with $j = r$. This is possible

for any allowed value of s . The degeneracy of this configuration is $g = \binom{K}{K-1} \binom{K}{s+1} = K \binom{K}{s+1}$. Thus,

$$g_1 = K \binom{K}{s+1} + K \binom{K}{s-1} ,$$

and thus for $r > 0$ and $s > 0$ we have

$$\begin{aligned} C(T) &= \frac{g_1}{g_0} k_B \left(\frac{\hbar\omega}{k_B T} \right)^2 e^{-\hbar\omega/k_B T} + \dots \\ &= K \cdot \left\{ \frac{K-s}{s+1} + \frac{s}{K-s+1} \right\} \cdot k_B \left(\frac{\hbar\omega}{k_B T} \right)^2 e^{-\hbar\omega/k_B T} + \dots \end{aligned}$$

The situation is depicted in Fig. 4. Upon reflection, it becomes clear that this expression is also valid for $s = 0$, since the second term in the curly brackets in the above equation, which should be absent, yields zero anyway.

The exceptional cases occur when $r = 0$, in which case there is no $j = r - 1$ level to depopulate. In this case, $g_1 = K \binom{K}{s-1}$ and $g_1/g_0 = Ks/(K - s + 1)$. Note that all our results are consistent with the $K = 2$ case studied earlier.

(5.15) A noninteracting Bose gas in $d = 3$ dimensions has dispersion $\varepsilon(\mathbf{k}) = \hbar c|\mathbf{k}|$.

- (a) Find $T_c(n)$.
- (b) For $T < T_c$, find $n(T, n_0)$ and $p(T)$.
- (c) For $T > T_c$, find $n(T, z)$ and $p(T, z)$.
- (d) Find and plot the molar heat capacity at constant volume as a function of T/T_c . Comment on its noteworthy features.

Solution :

(a) The density of states is obtained from $g(\varepsilon) d\varepsilon = \frac{d^3k}{(2\pi)^3}$, which yields

$$g(\varepsilon) = \frac{\varepsilon^2}{2\pi^2(\hbar c)^3} .$$

The critical temperature is then determined by

$$n = \int_0^\infty d\varepsilon \frac{g(\varepsilon)}{e^{\varepsilon/k_B T_c} - 1} = \frac{\zeta(3)}{\pi^2} \left(\frac{k_B T_c}{\hbar c} \right)^3 ,$$

hence

$$T_c(n) = \frac{\hbar c}{k_B} \left(\frac{\pi^2 n}{\zeta(3)} \right)^{1/3} .$$

One has $\zeta(3) \approx 1.2020569$.

(b) For $T < T_c$, we have

$$n(T, n_0) = n_0 + \frac{\zeta(3)}{\pi^2} \left(\frac{k_B T}{\hbar c} \right)^3$$

$$p(T) = \frac{\zeta(4)}{\pi^2} \frac{(k_B T)^4}{(\hbar c)^3} .$$

One has $\zeta(4) = \frac{\pi^4}{90} \approx 1.0823232$.

(c) For $T > T_c$, we have

$$n(T, z) = \frac{1}{\pi^2} \left(\frac{k_B T}{\hbar c} \right)^3 \text{Li}_3(z)$$

$$p(T, z) = \frac{1}{\pi^2} \frac{(k_B T)^4}{(\hbar c)^3} \text{Li}_4(z) .$$

(d) The energy is given by $E - \mu N = -\frac{\partial}{\partial \beta} \ln \Xi$. With $\ln \Xi = -\beta \Omega = \beta pV$, the energy for $T > T_c$ is

$$E(T, V, z) = \mu N - V \frac{\partial}{\partial \beta} (\beta p)$$

$$= \frac{3V}{\pi^3} \frac{(k_B T)^4}{(\hbar c)^3} \text{Li}_4(z) .$$

The particle number for $T > T_c$ is

$$N(T, V, z) = \frac{V}{\pi^2} \left(\frac{k_B T}{\hbar c} \right)^3 \text{Li}_3(z) \quad .$$

When $T < T_c$, we have

$$E(T, V) = \frac{3 \zeta(4) V}{\pi^3} \frac{(k_B T)^4}{(\hbar c)^3} \quad , \quad N(T, V, n_0) = V n_0 + \frac{\zeta(3) V}{\pi^2} \left(\frac{k_B T}{\hbar c} \right)^3 \quad .$$

We may now compute $c_{V,N}$, the molar heat capacity at constant volume. For $T < T_c$,

$$c_{V,N}(T, z) = \frac{N_A}{N} \left(\frac{\partial E}{\partial T} \right)_{V,N} = \frac{12 \zeta(4)}{\zeta(3)} \left(\frac{T}{T_c(n)} \right)^3 R \quad .$$

For $T > T_c$, we write

$$dN|_V = \frac{3V}{\pi^2} \left(\frac{k_B T}{\hbar c} \right)^3 \text{Li}_3(z) \frac{dT}{T} + \frac{V}{\pi^2} \left(\frac{k_B T}{\hbar c} \right)^3 \text{Li}_2(z) \frac{dz}{z} \quad ,$$

so setting $dN|_V = 0$ requires a relation between dz and dT , viz.

$$\frac{dz}{z} = -\frac{dT}{T} \cdot \frac{3 \text{Li}_3(z)}{\text{Li}_2(z)} \quad .$$

We next differentiate the energy E , obtaining

$$\begin{aligned} dE|_V &= \frac{12 k_B}{\pi^2} V \left(\frac{k_B T}{\hbar c} \right)^3 \text{Li}_4(z) dT + \frac{3}{\pi^2} \frac{(k_B T)^4}{(\hbar c)^3} \text{Li}_2(z) \frac{dz}{z} \\ &= \frac{3 k_B}{\pi^2} V \left(\frac{k_B T}{\hbar c} \right)^3 \left\{ 4 \text{Li}_4(z) - \frac{3 \text{Li}_3^2(z)}{\text{Li}_2(z)} \right\} dT \quad . \end{aligned}$$

Thus, dividing through by dT and then by N/N_A ,

$$c_{V,N}(T, z) = 3R \left[\frac{4 \text{Li}_4(z)}{\text{Li}_3(z)} - \frac{3 \text{Li}_3(z)}{\text{Li}_2(z)} \right] \quad ,$$

along with

$$n(T, z) = \frac{1}{\pi^2} \left(\frac{k_B T}{\hbar c} \right)^3 \text{Li}_3(z) \quad \Rightarrow \quad \text{Li}_3(z) = \zeta(3) \left(\frac{T_c(n)}{T} \right)^3 \quad .$$

Note that $z \rightarrow 0$ as $T \rightarrow \infty$, in which case $c_{V,N} \rightarrow 3R$, which is the appropriate Dulong-Petit result for the case of a linear dispersion in $d = 3$ dimensions.

One remarkable aspect to our result is that

$$\begin{aligned} \lim_{T \rightarrow T_c^-(n)} c_{V,N}(T) &= \frac{12 \zeta(4)}{\zeta(3)} R \approx 10.80471 R \\ \lim_{T \rightarrow T_c^+(n)} c_{V,N}(T) &= \left[\frac{12 \zeta(4)}{\zeta(3)} - \frac{9 \zeta(3)}{\zeta(2)} \right] R \approx 4.227845 R \quad , \end{aligned}$$

which says that $c_{V,N}(T)$ exhibits a *discontinuous drop* at the critical temperature $T_c(n)$.

(5.16) Consider free fermions with density of states $g(\varepsilon) = A \varepsilon^\alpha$ and number density n .

- (a) Find the Fermi energy $\varepsilon_F(n)$.
- (b) Find the chemical potential shift at finite temperature up to terms of order T^4 .
- (c) Find the heat capacity at constant volume $C_{V,N}$ to first order in T .

Solution :

(a) We have

$$n = \int_0^{\varepsilon_F} d\varepsilon g(\varepsilon) = \frac{A \varepsilon_F^{\alpha+1}}{\alpha+1} \Rightarrow \varepsilon_F = \left(\frac{(\alpha+1)n}{A} \right)^{\frac{1}{\alpha+1}} .$$

(b) Invoking the Sommerfeld expansion,

$$n = \int_0^{\varepsilon_F} d\varepsilon g(\varepsilon) + \frac{\pi^2}{6} g'(\varepsilon_F) (k_B T)^2 + \frac{7\pi^4}{360} g'''(\varepsilon_F) (k_B T)^4 + \dots$$

We now write $\mu = \varepsilon_F + \delta\mu$ and solve for $\delta\mu(\varepsilon_F, T)$, using $n = \int_0^{\varepsilon_F} d\varepsilon g(\varepsilon)$. We write the double power series expansion of the above result, up to orders $(k_B T)^4$ and $(k_B T)^2 \delta\mu$:

$$0 = g(\varepsilon_F) \delta\mu + \frac{1}{2} g'(\varepsilon_F) (\delta\mu)^2 + \frac{\pi^2}{6} g'(\varepsilon_F) (k_B T)^2 + \frac{\pi^2}{6} g''(\varepsilon_F) (k_B T)^2 \delta\mu + \frac{7\pi^4}{360} g'''(\varepsilon_F) (k_B T)^4 + \dots$$

We now solve for the coefficients of the order $(k_B T)^2$ and $(k_B T)^4$ terms in $\delta\mu(T)$, yielding

$$\delta\mu(T) = -\frac{\pi^2}{6} \frac{g'(\varepsilon_F)}{g(\varepsilon_F)} (k_B T)^2 - \frac{\pi^4}{360} \left\{ \frac{7g'''(\varepsilon_F)}{g(\varepsilon_F)} - \frac{10g'(\varepsilon_F)g''(\varepsilon_F)}{g^2(\varepsilon_F)} + \frac{5g'^3(\varepsilon_F)}{g^3(\varepsilon_F)} \right\} (k_B T)^4 + \dots$$

Substituting $g(\varepsilon) = A \varepsilon^\alpha$ into the above expression, we find

$$\delta\mu(T) = -\frac{\alpha\pi^2}{6} \frac{(k_B T)^2}{\varepsilon_F} - \frac{\alpha(\alpha-2)(2\alpha-7)\pi^4}{360} \frac{(k_B T)^4}{\varepsilon_F^3} + \dots$$

(c) The heat capacity is

$$C_{V,N} = \frac{\pi^2}{3} V g(\varepsilon_F) k_B^2 T = \frac{\pi^2}{3} V A \varepsilon_F^\alpha k_B^2 T \quad ,$$

where $\varepsilon_F(n)$ is given in the solution to part (a).

(5.17) In an n -type semiconductor, the donor levels lie a distance Δ below the bottom of the conduction band. Suppose there are M such donor levels. Due to the fact that such donor levels are spatially localized, one can ignore the possibility of double occupancy. Thus, each donor level can be occupied by at most one electron, but of either spin polarization. Assume the conduction band dispersion is isotropic, given by $\varepsilon_{\mathbf{k}} = \hbar^2 \mathbf{k}^2 / 2m^*$. You may set the conduction band minimum to $\varepsilon_c(0) \equiv 0$.

- Assuming that the conduction band is very sparsely populated, find an expression for the conduction electron density $n_c(T, \mu)$.
- Suppose there are N_d electrons sitting on the donor sites, *i.e.* N_d of the M donor levels are singly occupied. Find the entropy of these electrons.
- Find the chemical potential of the donor electrons.
- Use the fact that the donor electrons and the conduction band electrons are in thermal equilibrium to eliminate μ from the problem, and find the conduction electron density $n_c(T)$ and the fraction $\nu_d(T)$ of occupied donor sites. Assume that the donor concentration is ρ_d , and that all conduction electrons are due to singly ionized donors.

Solution :

(a) We have

$$n_c = 2 \int \frac{d^3k}{(2\pi)^d} \frac{1}{e^{\beta(\varepsilon_{\mathbf{k}} - \mu_c)} + 1} \approx 2\lambda_c^{-3} e^{\mu_c/k_B T} \quad ,$$

where μ_c is the chemical potential and $\lambda_c = (2\pi\hbar^2/m^*k_B T)^{1/2}$ thermal de Broglie wavelength for the conduction electrons.

(b) We assume that each donor site can either be empty, or else occupied by an electron in one of two possible polarization states. We forbid double occupancy of the donors, due to the large Coulomb energy associated with such a state. The number of configurations for N_d occupied donor sites is then

$$\Omega(N_d, M) = 2^{N_d} \binom{M}{N_d} \quad ,$$

and therefore

$$S_d = k_B \ln \left(\frac{2^{N_d} M!}{N_d! (M - N_d)!} \right) \quad .$$

The free energy of the donor system is then

$$\begin{aligned} F(T, N_d, M) &= -N_d \Delta - k_B T \ln \left(\frac{2^{N_d} M!}{N_d! (M - N_d)!} \right) \\ &\approx -N_d \Delta - N_d k_B T \ln 2 + M k_B T \left\{ \frac{N_d}{M} \ln \left(\frac{N_d}{M} \right) + \left(\frac{M - N_d}{M} \right) \ln \left(\frac{M - N_d}{M} \right) \right\} \quad , \end{aligned}$$

where we have invoked Stirling's approximation. The chemical potential for the donor level electrons, which we will need later, is then

$$\mu_d = \left(\frac{\partial F}{\partial N_d} \right)_{T, M} = -\Delta - k_B T \ln 2 + k_B T \ln \left(\frac{f_d}{1 - f_d} \right) \quad ,$$

where $f_d = N_d/M$ is the fraction of donor sites which are occupied.

(c) Invoking our results from part (a) and (b), and setting $\mu_c = \mu_d \equiv \mu$, we have

$$e^{\mu/k_B T} = \frac{1}{2} n_c \lambda_c^3 = \frac{1}{2} e^{-\Delta/k_B T} \frac{f_d}{1 - f_d} \quad ,$$

Thus,

$$(f_d^{-1} - 1) n_c = \lambda_c^{-3} e^{-\Delta/k_B T} \quad .$$

Now suppose the donor site density is ρ_d . All the conduction electrons must come from ionized donor sites. The fraction of such sites is $1 - f_d$, hence $n_c = (1 - f_d) \rho_d$. Therefore, we have

$$\frac{(1 - f_d)^2}{f_d} = \frac{e^{-\Delta/k_B T}}{\rho_d \lambda_c^3} \equiv b(T) \quad .$$

This yields a quadratic equation for $1 - f_d$, whose solution is

$$1 - f_d = -\frac{1}{2}b + \sqrt{\frac{1}{4}b^2 + b} \quad \Rightarrow \quad n_c = \left\{ -\frac{1}{2}b + \sqrt{\frac{1}{4}b^2 + b} \right\} \rho_d \quad .$$

Note that $f_d \rightarrow 1$ as $b \rightarrow 0$. In this limit, which is achieved when $k_B T \ll \Delta$, or when $\rho_d \lambda_c^3 \gg 1$, or by some combination of these two conditions, all the donor sites are occupied, and the conduction electron density is zero. It is energetically/entropically too costly for the donors to donate an electron to the conduction band. In the $T \rightarrow 0$ limit, we have $1 - f_d \simeq \sqrt{b}$, hence the chemical potential becomes

$$\mu(T \rightarrow 0) = -\frac{1}{2}\Delta + k_B T \ln \left[\frac{1}{2} \rho_d \left(\frac{2\pi\hbar^2}{m^* k_B T} \right)^{3/2} \right] \quad ,$$

which ultimately ends up exactly halfway between the donor levels and the bottom of the conduction band.

This problem is very similar to the adsorption model considered in ch. 4 of the lecture notes. There, we considered a surface of adsorption sites in equilibrium with a classical gas. The only difference here is that the adsorbate particles can exist in one of two energetically degenerate polarization states. One can also solve for the donor density in the grand canonical ensemble. The donors are independent, hence the partition function for the donor electrons is

$$\Xi_d = (1 + 2 e^{\mu/k_B T} e^{\Delta/k_B T})^M \quad .$$

Note the factor of two, due to the degeneracy of the spin polarization states. If we were to include the possibility of doubly occupied donors, we would have instead

$$\Xi_d = (1 + 2 e^{\mu/k_B T} e^{\Delta/k_B T} + e^{2\mu/k_B T} e^{(2\Delta-U)/k_B T})^M \quad ,$$

where the energy of the doubly occupied level is $-2\Delta + U$, with U being the Coulomb repulsion energy for two electrons to sit on the same localized donor site. Again, we have assumed U is much larger than every other energy scale in this problem, meaning we can ignore the possibility of double occupancy. The grand potential for the donor electrons is then $\Omega_d = -k_B T \ln \Xi_d$, and so

$$f_d = -\frac{1}{M} \left(\frac{\partial \Omega_d}{\partial \mu} \right)_{T,M} = \frac{1}{\frac{1}{2} e^{-(\mu+\Delta)/k_B T} + 1} \quad ,$$

which recovers the result previously obtained in part (a).