28

Bose–Einstein Statistics

The world is full of magical things patiently waiting for our wits to grow sharper.

Bertrand Russell (1872–1970), philosopher and mathematician

Perhaps the most startling property of systems governed by Bose–Einstein statistics is that they can exhibit a phase transition in the absence of interactions between the particles. In this chapter we will explore the behavior of an ideal gas of bosons and show how this unusual phase transition arises.

28.1 Basic Equations for Bosons

We begin with the Bose–Einstein equations for N and U, taken from eqs. (27.55) and (27.56),

$$N = \sum_\alpha \langle n_\alpha \rangle = \sum_\alpha (\exp[\beta(\epsilon_\alpha - \mu)] - 1)^{-1} \tag{28.1}$$

$$U = \sum_\alpha \epsilon_\alpha \langle n_\alpha \rangle = \sum_\alpha \epsilon_\alpha (\exp[\beta(\epsilon_\alpha - \mu)] - 1)^{-1}. \tag{28.2}$$

We are interested in understanding experiments in which the chemical potential μ is unknown and the number of particles N is fixed. On the other hand, as discussed in Chapter 27, eqs. (28.1) and (28.2) were derived under the assumption that μ is known. This leads us to begin calculations by finding $N = N(T, \mu)$ from eq. (28.1), and then inverting the equation to obtain the chemical potential, $\mu = \mu(T, N)$. After we have found μ, we can use eq. (28.2) to calculate the energy and the specific heat for a fixed number of particles.

28.2 $\langle n_\alpha \rangle$ for Bosons

The occupation number for bosons was derived in Chapter 27 and given in eq. (27.50),

$$f_{BE}(\epsilon_\alpha) = \langle n_\alpha \rangle = (\exp[\beta(\epsilon_\alpha - \mu)] - 1)^{-1}. \tag{28.3}$$

Although the expressions for the occupation numbers for bosons and fermions only differ by a plus or minus sign in the denominator, the consequences of this small difference are enormous. The first consequence of the minus sign in the denominator of eq. (28.3) for bosons is a limitation on the allowed values of the chemical potential. Since $f_{BE}(\epsilon_\alpha)$ gives the average number of particles in a single-particle state with energy ϵ_α, it cannot be negative,

$$(\exp[\beta(\epsilon_\alpha - \mu)] - 1)^{-1} > 0. \tag{28.4}$$

This immediately requires that

$$\epsilon_\alpha > \mu, \tag{28.5}$$

for *all* values of ϵ_α. In particular, if $\epsilon_\alpha = 0$ is the lowest energy of a single-particle state, then

$$\mu < 0. \tag{28.6}$$

The chemical potential of a gas of bosons must be negative.

Eq. (28.6) is *almost* a general result. It assumes that the lowest energy level is zero, which might not always be true. Because this can be a trap for the unwary, it is very important to know *why* μ is algebraically less than the energy of the lowest single-particle state, instead of just remembering that it is less than zero.

28.3   The Ideal Bose Gas

For systems with a continuous energy spectrum, we expect to be able to change the sums in eqs. (28.1) and (28.2) into integrals and use eqs. (27.61) and (27.62) to calculate the properties of the system. For bosons, these equations take the following form:

$$N = \int_0^\infty D_{BE}(\epsilon) \left(\exp[\beta(\epsilon - \mu)] - 1\right)^{-1} d\epsilon \tag{28.7}$$

$$U = \int_0^\infty D_{BE}(\epsilon) \, \epsilon \left(\exp[\beta(\epsilon - \mu)] - 1\right)^{-1} d\epsilon. \tag{28.8}$$

A particularly important case, which we will discuss in detail, is an ideal gas of bosons. We have already derived the single-particle density of states for particles in a box in eq. (27.13),

$$D_{BE}(\epsilon) = \frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\epsilon^{1/2}. \tag{28.9}$$

Eq. (28.9) completes the equations we need to investigate the properties of free bosons. We will begin to calculate those properties by looking at the low-temperature behavior of the chemical potential in the next section.

28.4   Low-Temperature Behavior of μ

We can simplify the problem of finding the chemical potential from eq. (28.7) by making the integral dimensionless. To do this, we introduce a dimensionless variable $x = \beta\epsilon$,

$$N = \int_0^\infty \frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\epsilon^{1/2}\left(\exp[\beta(\epsilon-\mu)]-1\right)^{-1}d\epsilon \tag{28.10}$$

$$= \frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}(k_BT)^{3/2}\int_0^\infty x^{1/2}\left(\exp(-\beta\mu)\exp(x)-1\right)^{-1}dx.$$

It is convenient at this point to introduce the fugacity

$$\lambda = \exp(\beta\mu). \tag{28.11}$$

Note that because $\mu < 0$, the fugacity must be less than 1, and its reciprocal, which enters into eq. (28.10), must be greater than 1,

$$\lambda^{-1} > 1 \tag{28.12}$$

In terms of the fugacity, the equation for N becomes

$$N = \frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}(k_BT)^{3/2}\int_0^\infty x^{1/2}\left(\lambda^{-1}\exp(x)-1\right)^{-1}dx. \tag{28.13}$$

The form of eq. (28.13) is extremely important in understanding the properties of bosons. As the temperature is decreased, the factor of $T^{3/2}$ in front of the integral also decreases. Since the total number of particles is fixed, the dimensionless integral in eq. (28.13) must increase. The only parameter in the integral is the inverse fugacity, so it must vary in such a way as to increase the value of the integral. Since the inverse fugacity is in the denominator of the integrand, the only way to increase the value of the integral is to decrease the value of the inverse fugacity. However, because of eq. (28.12) we cannot decrease the value of the inverse fugacity below $\lambda^{-1} = 1$. If the value of the dimensionless integral in eq. (28.13) diverged as $\lambda^{-1} \to 1$, there would be no problem.

However, although the *integrand* diverges at $x = 0$ when $\lambda = 1$, the value of the integral is finite:

$$\int_0^\infty x^{1/2} \left(\exp(x) - 1\right)^{-1} dx = \frac{\sqrt{\pi}}{2} \zeta\left(\frac{3}{2}\right) = 1.306\sqrt{\pi} = 2.315. \tag{28.14}$$

It is traditional to express the value of the integral in eq. (28.14) in terms of a ζ-function instead of simply 2.315. This is largely because the theory of bosons was developed before computers were available. At that time, instead of simply evaluating integrals numerically, great efforts were made to express them in terms of 'known' functions; that is, functions whose values had already been tabulated. Although retaining the ζ-function is a bit of an anachronism, I have included it and the factor of $\sqrt{\pi}$ in eq. (28.14) in the following equations for the sake of tradition (and comparison with other textbooks).

The consequence of the dimensionless integral in eq. (28.14) having an upper bound is that the equation cannot be correct below a temperature T_E that is determined by setting the integral equal to its maximum value,

$$N = \frac{V}{4\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} (k_B T_E)^{3/2} 1.306\sqrt{\pi}. \tag{28.15}$$

This equation can also be written as

$$N = 2.315 \frac{V}{4\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} (k_B T_E)^{3/2}. \tag{28.16}$$

The temperature T_E is known as the Einstein temperature,

$$k_B T_E = \left(\frac{2\pi\hbar^2}{m}\right) \left(\frac{N}{2.612\,V}\right)^{2/3}. \tag{28.17}$$

For fixed N and temperatures less than T_E, eq. (28.13) has no solution, even though you can certainly continue to cool a gas of bosons below T_E. This apparent contradiction has an unusual origin. Even though the energy levels are very closely spaced, so that changing from a sum in eq. (28.1) to the integral in eq. (28.7) would not normally be expected to cause difficulties, eq. (28.7) is not valid for $T < T_E$.

In the next section we will show how to remove the contradiction by modifying eq. (28.7) to treat the lowest energy state explicitly.

28.5 Bose–Einstein Condensation

We can trace the strange behavior of bosons at low temperatures to the form of the boson occupation number in eq. (28.3),

$$f_{BE}(\epsilon) = \langle n_\epsilon \rangle = (\exp[\beta(\epsilon - \mu)] - 1)^{-1}. \tag{28.18}$$

The difficulty arises from the fact that the occupation of the lowest energy level, $\epsilon = 0$, has an occupation number

$$f_{BE}(0) = \langle n_0 \rangle = N_0 = (\exp[-\beta\mu] - 1)^{-1}. \tag{28.19}$$

If we were to set $\mu = 0$, the occupation number would be infinite. This means that for very small but non-zero values of μ, the occupation number of the $\epsilon = 0$ state can be arbitrarily large. In fact, it can even contain all the bosons in the system!

As will be justified in Section 28.8, the only modification we need to make in eq. (28.7) is to include the number of particles in the $\epsilon = 0$ state, which we denote as N_0,

$$N = N_0 + \int_0^\infty D_{BE}(\epsilon) \, (\exp[\beta(\epsilon - \mu)] - 1)^{-1} \, d\epsilon. \tag{28.20}$$

For free bosons this becomes

$$N = N_0 + \frac{V}{4\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} (k_B T)^{3/2} \int_0^\infty x^{1/2} \left(\lambda^{-1} \exp(x) - 1\right)^{-1} dx. \tag{28.21}$$

Above the temperature T_E, the occupation N_0 of the $\epsilon = 0$ state is much smaller than the total number N of particles in the system, and may be neglected. Below T_E, the value of N_0 is comparable to N. That is, a significant fraction of the particles in the system are in the single-particle state with the lowest energy. The transition at T_E is called the Bose–Einstein condensation, because a significant fraction of the particles 'condense' into the $\epsilon = 0$ state at temperatures below T_E.

28.6 Below the Einstein Temperature

The behavior of the Bose gas below T_E turns out to be remarkably simple and easy to calculate. If we compare eq. (28.21) with eq. (28.15), which determines the Einstein temperature, we see that we can rewrite eq. (28.21) as

$$N = N_0 + N \left(\frac{T}{T_E} \right)^{3/2}. \tag{28.22}$$

We can then solve this equation for the occupation of the $\epsilon = 0$ state below T_E,

$$N_0 = N \left[1 - \left(\frac{T}{T_E} \right)^{3/2} \right]. \tag{28.23}$$

Eq. (28.23) shows that $N_0 \to N$ as $T \to 0$; for zero temperature all particles are in the lowest single-particle energy state.

Eq. (28.23) also shows that as $T \to T_E$, $N_0 \to 0$. This result is, of course, only an approximation. What it means is that above T_E, $N_0 \ll N$, so that it can be safely ignored.

Note that as $T \to T_E$ from eq. (28.24), N_0 goes linearly to zero:

$$\frac{N_0}{N} = \frac{3}{2} \left(\frac{T_E - T}{T_E} \right) + \cdots. \tag{28.24}$$

If we combine eq. (28.23) with eq. (28.19), we can find the temperature dependence of the chemical potential (taking the lowest single-particle energy state to be zero)

$$N_0 = [\exp(-\beta\mu) - 1]^{-1} = N \left[1 - \left(\frac{T}{T_E} \right)^{3/2} \right]. \tag{28.25}$$

Since we know that $\beta\mu$ is very small below T_E, we can expand $\exp(-\beta\mu)$ in eq. (28.25) to find a very good approximation for μ,

$$\mu \approx -\frac{k_B T}{N} \left[1 - \left(\frac{T}{T_E} \right)^{3/2} \right]^{-1}. \tag{28.26}$$

Because of the factor of $1/N$ in eq. (28.26), the chemical potential μ is extremely small below the Einstein temperature T_E; if N is of the order of Avogadro's number, $|\mu|$ is smaller than $10^{-23} k_B T$.

The approximation in eq. (28.26) also shows that as $T \to T_E$, the value of μ falls sharply. If T is close enough to the Einstein temperature, the approximation breaks down. However, this only happens when T is extremely close to T_E. For all practical purposes, eq. (28.26) can be used for all temperatures below T_E.

Now that we have found the chemical potential for an ideal gas of bosons, we are in a position to calculate the energy and the specific heat, which we will do in the next section.

28.7 Energy of an Ideal Gas of Bosons

Given the chemical potential, we can calculate the energy of a gas of bosons from eq. (28.8),

$$U = U_0 + \int_0^\infty D_{BE}(\epsilon)\,\epsilon\,(\exp[\beta(\epsilon - \mu)] - 1)^{-1}\,\epsilon\,d\epsilon. \tag{28.27}$$

In this equation,

$$U_0 = 0 \tag{28.28}$$

is the energy of a particle in the lowest energy level is $\epsilon = 0$.

Introducing the dimensionless variable $x = \beta\epsilon$, as we did in eq. (28.13), we can write an equation for U in terms of a dimensionless integral

$$U = \frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}(k_B T)^{5/2}\int_0^\infty x^{3/2}\left(\lambda^{-1}\exp(x) - 1\right)^{-1}dx. \tag{28.29}$$

Below T_E, eq. (28.29) simplifies because $\lambda^{-1} = 1$. The dimensionless integral can be evaluated numerically,

$$\int_0^\infty x^{3/2}\,(\exp(x) - 1)^{-1}\,dx = \zeta\left(\frac{5}{2}\right)\Gamma\left(\frac{5}{2}\right) = 1.341\left(\frac{3}{4}\right)\pi^{1/2} = 1.7826. \tag{28.30}$$

In this equation, $\Gamma(\cdot)$ indicates the gamma function and $\zeta(\cdot)$ again indicates the zeta function.

Using eq. (28.30), eq. (28.29) becomes

$$U = 1.7826\frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}(k_B T)^{5/2}. \tag{28.31}$$

Since we know from eq. (28.15) that

$$N = 2.315\frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}(k_B T_E)^{3/2}, \tag{28.32}$$

we find that the energy per particle has a simple form,

$$\frac{U}{N} = \left(\frac{1.7826}{2.315}\right)\left(\frac{T}{T_E}\right)^{3/2}k_B T = .7700\left(\frac{T}{T_E}\right)^{3/2}k_B T. \tag{28.33}$$

The specific heat at constant volume is found by differentiating with respect to temperature,

$$c_V = 1.925 \, k_B \left(\frac{T}{T_E} \right)^{3/2}. \tag{28.34}$$

Notice that for $T = T_E$, the specific heat takes on the value of $1.925 \, k_B$, which is greater than the classical value of $1.5 \, k_B$ that it takes on in the limit of high temperatures.

For temperatures above T_E, the specific heat of an ideal boson gas decreases monotonically to its asymptotic value of $1.5 \, k_B$. The derivation involves expanding the integral in eq. (28.8) as a function of $\beta \mu$. Since the expansion involves interesting mathematics, but little physics, I will refer the readers to the many textbooks that give the details. The fastest and easiest way to obtain the function today is to carry out the integral in eq. (28.8) numerically, which will be done in Section 28.11.

28.8   What About the Second-Lowest Energy State?

Since we have seen that the occupation of the lowest energy level has such a dramatic effect on the properties of a gas of bosons, it might be expected that the second-lowest energy state would also play a significant role. Oddly enough, it does not, even though the second-lowest energy state lies only slightly higher than the lowest energy state.

The energy levels are given by eq. (27.7). Since the wave function in eq. (27.3) vanishes if n_x, n_y, or n_z is zero, the lowest energy level, ϵ_o, corresponds to $\vec{n} = (1, 1, 1)$. This gives us

$$\epsilon_0 = \epsilon_{(1,1,1)} = \frac{\hbar^2 \pi^2}{2mL^2} \left(1^2 + 1^2 + 1^2 \right) = 3 \frac{\hbar^2 \pi^2}{2mL^2}. \tag{28.35}$$

The next lowest energy level, ϵ_1, corresponds to $\vec{n} = (1, 1, 2)$, or $(1, 2, 1)$, or $(2, 1, 1)$ These three states each have the energy

$$\epsilon_1 = \epsilon_{(1,1,2)} = \frac{\hbar^2 \pi^2}{2mL^2} \left(1^2 + 1^2 + 2^2 \right) = 6 \frac{\hbar^2 \pi^2}{2mL^2}. \tag{28.36}$$

The difference in energy between the two states is

$$\Delta \epsilon = \epsilon_1 - \epsilon_0 = 3 \frac{\hbar^2 \pi^2}{2mL^2}. \tag{28.37}$$

The energy difference found in eq. (28.37) is extremely small. Suppose we consider a system consisting of ^4He in a cubic container with $L = 1 \, cm$. The energy difference is only about $2.5 \times 10^{-26} \, erg$. Expressing this as a temperature, we have

$$\frac{\Delta\epsilon}{k_B} \approx 1.8 \times 10^{-14} K. \tag{28.38}$$

Despite the fact that this energy difference is so small, it has a large effect on the occupation number of the state because it is substantially larger than the difference between the chemical potential and the lowest single-particle energy level.

Define $\tilde{\mu} = \mu - \epsilon_0$ as the difference between the chemical potential and the lowest single-particle energy level. This will allow us to use eq. (28.26) with only the substitution $\mu \to \tilde{\mu}$.

From eq. (28.26) we see that $\beta\tilde{\mu} \approx -1/N \approx -10^{-23}$, so that the occupation number, $\langle n_1 \rangle$, of the second-lowest energy levels is

$$\langle n_1 \rangle = (\exp(\beta(\Delta\epsilon - \tilde{\mu})) - 1)^{-1} \tag{28.39}$$

$$\approx (\exp(\beta\Delta\epsilon) - 1)^{-1}$$

$$\approx \frac{1}{\beta\Delta\epsilon}$$

$$\approx \frac{T}{1.8 \times 10^{-14} K},$$

$$\approx (5.5 \times 10^{13} K^{-1})T,$$

where the last two lines come from eq. (28.38). The occupation of the second lowest states is of the order of 10^{12} or more, but this is still very small in comparison to the total number of particles, $N \approx 10^{23}$, or the number of particles in the lowest energy state below T_E. Because the numbers of particles in each of the states above the lowest-energy state are so much smaller than the number in the lowest-energy state, it is completely sufficient to use the integral in eq. (28.20) to calculate their total contribution.

28.9   The Pressure below $T < T_E$

Eq. (27.65) has an interesting consequence for the pressure of a boson gas below the Bose–Einstein condensation. If we insert eq. (27.65) into eq. (28.31), we obtain

$$P = \frac{2}{3}\frac{U}{V} = 0.2971\frac{1}{\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}(k_B T)^{5/2}. \tag{28.40}$$

This means that the pressure along any isotherm for a gas of bosons below T_E is constant. It depends on the mass of the particles and the temperature, but nothing else. Another way of expressing this is to say that the isothermal compressibility of an ideal Bose gas is infinite below the Bose–Einstein transition.

28.10   Transition Line in *P-V* Plot

We can combine eq. (28.17) with eq. (28.40) to find the Bose–Einstein transition line in a *P-V* plot,

$$P = 0.9606\, \hbar^2 m \pi^{1/2} \left(\frac{N}{V}\right)^{5/3}. \tag{28.41}$$

As eq. (28.41) shows, the pressure is proportional to the (5/3)-power of the number density along the transition line.

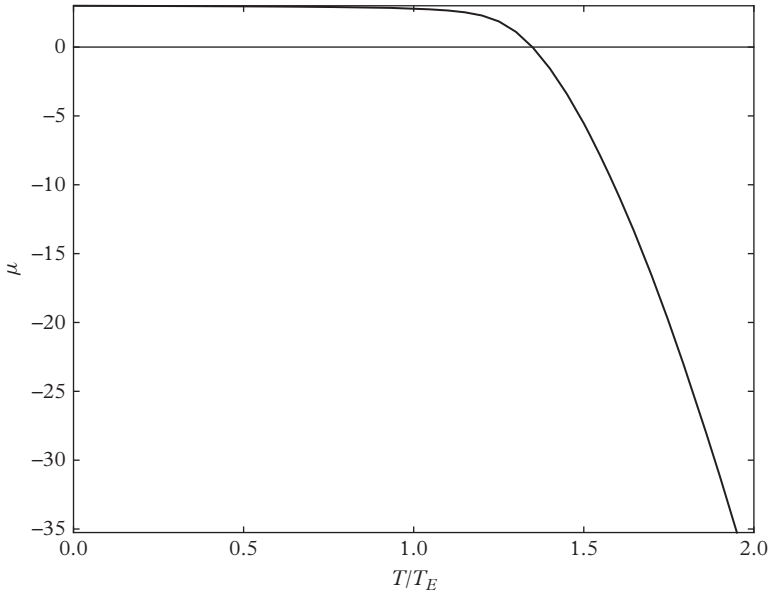## 28.11   A Numerical Approach to Bose–Einstein Statistics

This concludes the derivation of the integral equations describing the Bose–Einstein transition. The treatment is correct, but not entirely satisfying. The derivation jumps from the original equations involving discrete sums, eqs. (28.1) and (28.2), to new equations with the sums replaced by integrals, eqs. (28.7) and (28.8), then back to the sums to extract to lowest energy state, then back to the integrals for all higher energy states.

As an alternative, a completely numerical approach will be presented in the first five problems at the end of the chapter. The approach only involves the sums in eqs. (28.1) and (28.2). It was developed by a student, Tyson Price, and has appeared in the literature.[1] The alternative approach does not treat the lowest energy state differently than the rest. The large number of particles in the lowest energy state is simply a result of the numerical solution. Temperatures above and below the Einstein temperature are handled in the same way.
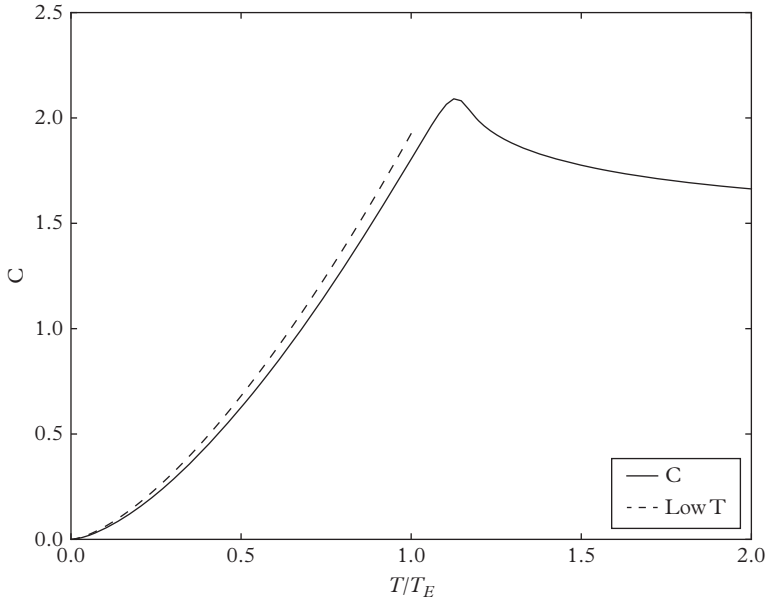
The inversion of the equation for the number of particles, $N = N(\mu, T)$, must also be performed numerically, because a solution for $\mu = \mu(N, T)$ is not available. This is the subject of Problem 28.2. A plot of μ as a function of temperature is shown in Fig. 28.1.

Problem 28.4 guides you through the calculation of the specific heat as a function of temperature. Fig. 28.2 shows a plot of the result for $N = 10000$, compared to a plot in the same figure of the analytic result of the low-temperature specific heat from eq. (28.34). The specific heat above T_E is considerably more difficult to obtain with an analytic approximation, but numerically it is easy. The plot for $N = 10000$ shows a smooth maximum, typical of a finite system. The height of the maximum is greater than
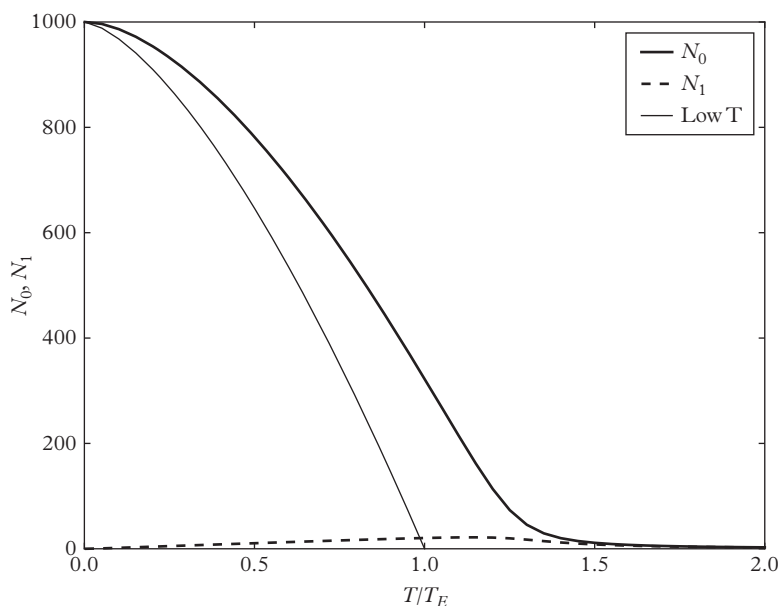
[1] T. Price, R. H. Swendsen, 'Numerical computation for teaching quantum statistics,' *Am. J. Phys.*, 81: 866–72 (2013). Earlier work by other authors treated bosons confined by harmonic traps: S. Grossmann and M. Holthaus, 'On Bose–Einstein condensation in harmonic traps,' *Phys. Lett.* A 208, 188–92 (1995). M. Ligare, 'Numerical analysis of Bose–Einstein condensation in a three-dimensional harmonic oscillator potential,' *Am. J. Phys.*, 66: 185–90 (1998). M. Ligare, 'Comment on "Numerical analysis of Bose–Einstein condensation in a three-dimensional harmonic oscillator potential"—An extension to anisotropic traps and lower dimensions,' *Am. J. Phys.*, 70: 76–8 (2002).

Fig. 28.1 *The chemical potential, μ, in units of $\hbar^2\pi^2/2mL^2 = \epsilon_0/3$ is plotted as a function of T/T_E for $N = 1000$ from the numerical calculation described in the text.*

Fig. 28.2 *The specific heat in units of k_B as a function of T/T_E for $N = 10000$ from the numerical calculation described in the text. The analytic low-temperature result is shown as a dashed line for comparison.*

Fig. 28.3 *The occupation numbers, N_0 and N_1, are plotted as a function of T/T_E for $N = 1000$ from the numerical calculation described in the text. The analytic low-temperature result, Eq. (28.19) for N_0 is shown for comparison.*

the specific heat at $T = T_E$, which is a finite-size effect. The height of the maximum is greatest for about $N = 1000$, and decreases for larger systems.

Problem 29.5 has you calculate the occupation of the two lowest single-particle states, and compare them to the asymptotic curves. A plot is shown in Fig. 28.3.

28.12　Problems

PROBLEM 28.1
Boson Gas Problem: Numerical computation of $N = N(\mu, T)$

Write a program to compute the average number of particles as a function of the chemical potential μ and the temperature T by direct summation without using the integral approximation.

Consider an ideal quantum gas of N particles, each with mass m, in a cubic box with sides of length L. The N-particle Hamiltonian is

$$H = \sum_{j=1}^{N} \frac{|\vec{p}_j|^2}{2m}.$$

The single-particle energy is

$$\epsilon(\vec{n}) = An^2,$$

where $\vec{n} = (n_x, n_y, n_z)$ and $n^2 = n_x^2 + n_y^2 + n_z^2$. The value of the constant A is

$$A = \frac{\hbar^2}{2m} \frac{\pi^2}{L^2},$$

but we will use dimensionless variables, with $A = 1$ and $k_B = 1$. [Your program should still contain the constants A and k_B in case we want to use values with dimensions in the future.]

The occupation number of a single-particle state with energy ϵ

$$\langle n_\epsilon \rangle = (\exp(\beta(\epsilon - \mu)) + \sigma)^{-1},$$

where for

$$
\begin{array}{ll}
Bose--Einstein & \sigma = -1 \\
Fermi--Dirac & \sigma = +1 \\
Maxwell--Boltzmann & \sigma = 0.
\end{array}
$$

Your program should contain σ as a parameter, so that you can treat any kind of statistics.

The basic equation for the average number of particles $\langle N \rangle$ (which can be written as N for simplicity) as a function of μ and T is

$$N(\mu, T) = \sum_{\vec{n}} \langle n_{\epsilon_{\vec{n}}} \rangle = \sum_{\vec{n}} (\exp(\beta(\epsilon(\vec{n}) - \mu)) + \sigma)^{-1}.$$

You will not need the equation for U for this assignment.

1. Since the sum in the equation for $N(\mu, T)$ is over an infinite number of terms, it must be truncated to a finite number of terms for the program. Find a criterion for truncating the sum such that the neglected terms are each smaller than some δ. In practice, you will find that you can choose $\delta = 10^{-8}$, or even smaller, without making the run time program too long.
2. Write a function using Python (or another programming language of your choice) to carry out the truncated sum in the equation for $N(\mu, T)$.
3. Write a loop using the function you programed in answer to the previous question to compute $N(\mu, T)$ for uniformly spaced values of μ between arbitrary values μ_1 and μ_2.
4. Include a plot of N vs. μ in your program for the values you've computed. For this assignment, plot individual points.
5. For the special case of bosons ($\sigma = -1$) and $T = 1$, run your program for 37 values of μ between -1.0 and 7.0 (in units of $A = 1$).
6. Are there any strange features of the results? If there are, can you explain them?
7. Why did I specify 37 values of μ instead of 36 in the previous problem?

PROBLEM 28.2
Boson Gas Problem: Numerical computation of $\mu = \mu(T,N)$

In the previous problem, you wrote a function to compute the average number of bosons, $N = \langle N \rangle$, given the temperature T and the chemical potential μ. In this assignment, you will invert the function $N = N(\mu, T)$ to compute $\mu = \mu(T,N)$.

We will only be considering bosons for this assignment, but write your program using the more general occupation number of a single-particle state with energy ϵ

$$\langle n_\epsilon \rangle = (\exp(\beta(\epsilon - \mu)) + \sigma)^{-1}.$$

To invert the equation $N = N(\mu, T)$ to find $\mu = \mu(N, T)$, we need the fact that N is a monotonically increasing function of μ, as found in the previous assignment.

The basic algorithm begins with a choice of interval $[\mu_-, \mu_+]$ large enough to contain the desired value of $\mu(T,N)$. Fortunately, the choice is not very delicate. We then follow an iterative procedure until we find a value of μ that gives the correct number of particles. The suggested criterion is that $|\mu_+ - mu_-| < \delta\mu$, where $\delta\mu \approx 10^{-4}$.

1. Calculate $\mu_{trial} = (\mu_- + \mu_+)/2$.
2. Calculate $N_{trial} = N(\mu_{trial}, T)$.
3. If $\quad N_{trial} > N \quad$ set $\mu_+ = \mu_{trial}$
   If $\quad N_{trial} < N \quad$ set $\mu_- = \mu_{trial}$
4. Check to see if $\mu_+ - \mu_- < \delta\mu$. If not, return to step 1.

QUESTIONS:

1. Write a VPython function to compute $\mu = \mu(T,N)$.
2. Write a loop using the function you programed in answer to the previous question to compute $\mu(T,N)$ for uniformly spaced values of T between arbitrary values of T_- and T_+.
3. Calculate the Einstein temperature as a function of the parameter A.
4. For $N = 5$, 50, and 500, use your program to compute $\mu(T)$ for uniformly spaced values of T between $T = 0$ and $T = 2T_E$, where T_E is estimated from the expression you found in answer to the previous question.

PROBLEM 28.3
Quantum Gas Problem: A thermodynamic identity

A quantity that we wish to compute and plot is the heat capacity at constant N and V

$$C_{V,N} = T\left(\frac{\partial S}{\partial T}\right)_{V,N} = \left(\frac{\partial U}{\partial T}\right)_{V,N}.$$

Keeping V constant is not a problem, we will ignore the volume dependence to simplify the notation, writing C_N when we really mean $C_{V,N}$.

The difficulty is that the natural quantity to calculate is

$$\left(\frac{\partial U}{\partial T}\right)_{\mu}.$$

QUESTIONS:

1. Prove the following thermodynamic identity.

$$C_N = \left(\frac{\partial U}{\partial T}\right)_{\mu} - \left(\frac{\partial U}{\partial \mu}\right)_{T}\left(\frac{\partial N}{\partial T}\right)_{\mu}\bigg/\left(\frac{\partial N}{\partial \mu}\right)_{T}$$

2. Find explicit expressions for all quantities on the right side of Eq. (1) in terms of sums over $\vec{n}$.

PROBLEM 28.4
Boson Gas Problem: The heat capacity of an ideal gas of bosons

Using the thermodynamic identity you derived in the previous problem, write a program to compute the specific heat at constant particle number as a function of temperature,

$$C_{V,N} = \left(\frac{\partial U}{\partial T}\right)_{V,N}.$$

Include the integral approximation to $C_N(T)$ in your plot for $T < T_E$. You can find the appropriate formula in the textbook.

As previously, you will find it helpful to write the computation of C_N as a function in Python. In fact, much of the code for the function can be copied from earlier programs.

Plot your results for T between zero and $4T_E$, for $N = 5$, $N = 50$, and $N = 500$.

PROBLEM 28.5
Boson Gas Problem: Comparisons with the large-N results

We have derived closed form equations for some properties of the Bose–Einstein ideal gas in the large-N limit. In particular, we found that below T_c, the occupation of the ground state is

$$N_0 = N\left(1 - \left(\frac{T}{T_E}\right)^{3/2}\right)$$

and the specific heat is

$$c_{V,N} = 1.925k_B\left(\frac{T}{T_E}\right)^{3/2}.$$

1. Modify a copy of your program to compute $\mu(T,N)$ to make a plot of the ground state occupation N_0 as a function of T. In this new plot, include a plot of eq. (28.12) for comparison.

   Make plots for at least two different numbers of particles to see how eq. (28.12) is approached as N is increased.

2. Modify a copy of your program to compute $c_N(T)$ to include a plot of eq. (28.12) for comparison.

   Make plots for at least two different numbers of particles to see how eq. (28.12) is approached as N is increased.

The temperature range in the new plots should again be from $T = 0$ to $T = 2T_E$, but the functions in eq. (28.12) and (28.12) should each only extend from $T = 0$ to $T = T_E$.

PROBLEM 28.6
Bosons in two dimensions

Consider an ideal boson gas in two dimensions. The N particles in the gas each have mass m and are confined to a box of dimensions $L \times L$.

1. Calculate the density of states for the two-dimensional, ideal Bose gas.
2. Calculate the Einstein temperature in two dimensions in terms of the given parameters and a dimensionless integral. You *do* have to evaluate the dimensionless integral.

PROBLEM 28.7
Bosons in two dimensions with a bound state

Consider a simple model of bosons in a system with a single bound state. To simplify the math, we will consider the problem in two-dimensions.

   If the boson is not in the bound state, it is a free particle in a two-dimensional box of length L. The density of states is a constant, $\mathscr{D}(\epsilon) = D$, for $\epsilon > 0$.

   [You do not have to evaluate D.]

   The boson binding potential is represented by a single, **non-degenerate** bound state with energy $-\epsilon_o < 0$, *below the band.*

   Assume that the number of bosons is $N >> 1$.

1. Write down the equation or equations that determine the chemical potential.
2. What is the limit on possible values of the chemical potential? Explain your answer.

   To simplify the algebra, assume that $N = \epsilon_o D$ for the following questions.
3. Calculate the Einstein transition temperature, T_E.
4. For temperatures below the Einstein temperature, calculate the occupation of the ground state as a function of temperature.
5. For $T < T_E$, calculate the chemical potential as a function of temperature.

PROBLEM 28.8
Bosons in four dimensions

Consider an ideal boson gas in four dimensions. The N particles in the gas each have mass m and are confined to a box of dimensions $L \times L \times L \times L$.

1. Calculate the density of states for the four-dimensional, ideal Bose gas.

2. Calculate the Einstein temperature in four dimensions in terms of the given parameters and a dimensionless integral. You do not have to evaluate the dimensionless integral.
3. Below the Einstein temperature, calculate the occupation number of the lowest-energy, single-particle state as a function of temperture, in terms of the Einstein temperature and the total number of particles.
4. Calculate the chemical potential below the Einstein temperature.

PROBLEM 28.9
Energy of an ideal Bose gas in four dimensions

Again consider an ideal boson gas in four dimensions. The N particles in the gas each have mass m and are confined to a box of dimensions $L \times L \times L \times L$. Calculate the energy and the specific heat as functions of temperature below the Einstein temperature.

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