

1 Introduction

In this course we will be dealing with many-body quantum physics. As usual, *many-body* means that we are going to look at systems made of *macroscopic* number of particles. This means we will have to use (hence— recall and revise) quantum mechanics, thermodynamics and statistical physics. We will also have to introduce a set of suitable techniques, which we will do as we move through the material. But before we get to technicalities, let's make a simple dimensional estimate: let's consider a gas and see under which conditions quantum mechanics becomes relevant.

Consider a vessel filled with a gas of some sort. A typical distance between particles, l , is related to the number density, n , via $n \sim 1/l^3$. Quantum mechanics provides us with other length scale, known as the *de Broglie wavelength*:

$$p = \frac{h}{\lambda}, \quad (1)$$

where p is momentum of a particle and h is the Planck's constant. The condition for applicability of classical mechanics is that λ is much less than all the other length scales— in particular, the gas is classical as long as

$$\lambda \ll l \sim n^{-1/3}. \quad (2)$$

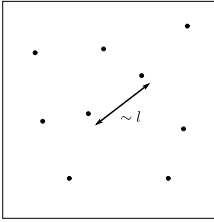


Figure 1: A cartoon of a vessel filled with gas. Here l stands for typical distance between particles.

It is easy to estimate a typical value of the de Broglie wavelength for an ideal (i.e., non-interacting) gas in thermal equilibrium at temperature T . Indeed, the typical energy scale per degree of freedom is $\epsilon \sim k_B T$, where k_B is the Boltzmann constant.¹ Typical kinetic energy of a molecule is of the same order of magnitude, $\epsilon \sim p^2/2m$, where m is a mass of a molecule. Therefore, we write $T \sim \epsilon \sim p^2/2m \sim (h/\lambda)^2/2m$, or, equivalently,

$$\lambda \sim \frac{h}{\sqrt{2mT}}. \quad (3)$$

The right-hand side of (3) is known as a *thermal wavelength*— it is nothing but a typical value of the de Broglie wavelength for a gas at a given temperature T .

Combining (2) and (3), we conclude that as long as

$$\frac{h}{\sqrt{2mT}} n^{1/3} \ll 1, \quad (4)$$

the gas behaves classically. Once this condition is violated, we are in the realm of quantum physics. For example:

- low T : ^4He becomes superfluid at $T_c \sim 1\text{K}$,
- small m : electrons in metals form a *Fermi liquid*,
- large density: in neutron stars, temperatures can reach $\sim 10^6\text{K}$, but the densities are so huge that the condition (4) is violated.

Before we can discuss any of these effects in any level of detail, we need to build an appropriate formalism: the so-called *second quantization*. We start by refreshing basic notions of quantum mechanics.

¹If temperature is measured in Kelvin and energy is Joules, then $k_B = 1.38 \times 10^{-23}\text{J/K}$. From now on I am going to measure temperature in the units of energy, so that in these units $k_B = 1$.

2 Quantization of a single particle motion

The wave function $\psi(x)$ of a particle of mass m moving in a potential $V(x)$ satisfies the Schrödinger equation

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x) + V(x)\psi(x) = E\psi(x) , \quad (5)$$

where E is the energy of the particle. Notice that we only consider one spatial dimension, otherwise x would be a vector, and instead of the second derivative we would have had the Laplace operator. The wave function is supposed to be normalized,

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1 . \quad (6)$$

Consider the so-called potential well,

$$V(x) = \begin{cases} 0, & 0 < x < L \\ \infty, & \text{otherwise.} \end{cases} \quad (7)$$

Here L is the width of the well. Since the well is infinitely deep, the particle cannot penetrate to the outside of the well, thus the wave function is only non-zero for $0 < x < L$. Hence, we shall solve the Schrödinger equation in the region $0 < x < L$ with the boundary conditions

$$\psi(0) = \psi(L) = 0 . \quad (8)$$

We seek the solutions to Eq. (5) in the form

$$\psi(x) = Ae^{i\lambda x} + Be^{-i\lambda x} , \quad (9)$$

where A , B and λ are some constants to be specified. Substituting this form of the wave function into (5), we find $E = \hbar^2 \lambda^2 / 2m$.

The boundary conditions yield:

$$x = 0 : \quad A + B = 0 \quad (10)$$

$$x = L : \quad Ae^{i\lambda L} + Be^{-i\lambda L} = 0 \quad (11)$$

There are two ways of fulfilling the above relations: either we set $A = 0$, which violates the normalization condition (6), or we require that $\lambda L = \pi l$, where $l = 1, 2, \dots$ is an integer. Notice that we do not allow for $l = 0$, since it would violate the normalization condition (6).

This way, we find a set of *single-particle states*, labelled by an integer l , which is usually called a *quantum number*. The energy of a particle in the state l is

$$E_l = \frac{\pi^2 \hbar^2}{2mL^2} l^2 , \quad (12)$$

and the wave function is $\psi_l(x) = A \sin(\pi l x / L)$. To find the value of the normalization constant A we plug this form of the wave function into (6):

$$1 = \int_{-\infty}^{\infty} |\psi_l(x)|^2 dx \quad (13)$$

$$= \int_0^L A^2 \sin^2 \pi l x / L dx \quad (14)$$

$$= A^2 \int_0^L \frac{1 - \cos 2\pi l x / L}{2} dx \quad (15)$$

$$= A^2 L / 2 . \quad (16)$$

Here in the second line we use the fact that $\psi_l(x) = 0$ for $x < 0$ and $x > L$, in the third line we used the identity $2 \sin^2 x = 1 - \cos 2x$. Finally we have

$$\psi_l(x) = \sqrt{\frac{2}{L}} \sin(\pi l \frac{x}{L}) . \quad (17)$$

Fig. (2) sketches wave functions (17) for $l = 1, 2, 3$.

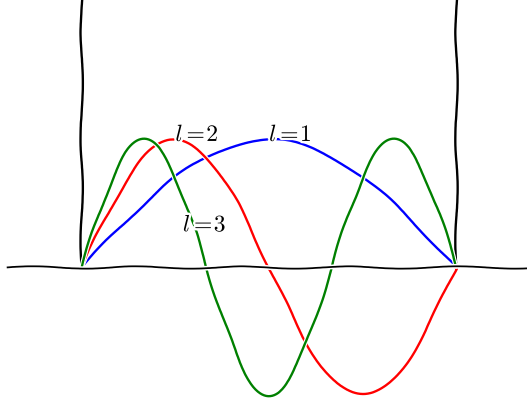


Figure 2: Wave functions (17).

The set of single-particle states (17) is by no means unique. First of all, different single-particle potentials $V(x)$ and different boundary conditions lead to different sets of single-particle states.

In general, from a set of single particle states we require that it is *orthonormal and complete*. Orthonormality means that (i) Each function of the set is normalized, and (ii) the functions with different quantum numbers are orthogonal to each other:

$$\int_{-\infty}^{\infty} \psi_l^*(x) \psi_{l'}(x) dx = \delta_{l,l'} , \quad (18)$$

where $\delta_{l,l'}$ is the Kronecker delta (1 if $l = l'$, and 0 if $l \neq l'$.)

It is easy to check that the set (17) is orthonormal: using the trigonometric identity $2 \sin x \sin y = \cos(x - y) - \cos(x + y)$, we find

$$\int_0^L \sin \pi l x / L \sin \pi l' x / L dx = 2 \int_0^L (\cos \pi(l - l')x / L - \cos \pi(l + l')x / L) dx = 0$$

unless $l = l'$.

Completeness of a set of states means that *any* single particle function which satisfies the given boundary conditions (e.g. (8)) can be expanded in terms of $\psi_l(x)$:

$$\psi(x) = \sum_l c(l) \psi_l(x) \quad (19)$$

where $c(l)$ are complex numbers.

The completeness condition can be written in a form similar to (18):

$$\sum_l \psi_l^*(x) \psi_l(x') = \delta(x - x') , \quad (20)$$

where $\delta(x)$ is the Dirac delta function.

Exercise 1 (*Periodic boundary conditions.*) Dealing with sine functions in (17) is often impractical. A more convenient set of states is constructed as follows: Consider the Schrödinger equation (5) again, but instead of the hard-wall boundary conditions (8) impose the so-called periodic boundary conditions

$$\psi(x) = \psi(x + L) . \quad (21)$$

1. Look for solutions in the form $\psi(x) = Ce^{ikx}$. Find the relation between k and E .
2. Impose the boundary conditions (21) and show that k must satisfy $kL = 2\pi l$ with $l = 0, \pm 1, \pm 2, \dots$.
3. Normalize the resulting wave functions using (6).
4. Check the orthonormality of the states using (18).
5. Check the completeness of the set of states using (20).

3 Two particles

Now as we understand a single-particle problem, suppose we put *two identical* particles (say, two electrons) into the potential well, Fig. 2. How do we go about this? The wave function now depends on two coordinates, $\Psi(x_1, x_2)$, and its normalization condition is

$$\int dx_1 dx_2 |\Psi(x_1, x_2)|^2 = 1 . \quad (22)$$

The wave functions must satisfy the Schrödinger equation, $\hat{H}\Psi = E\Psi$, where the Hamiltonian is the sum of kinetic energies and potential energies of both particles:

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x_1^2} - \frac{\hbar^2}{2m} \frac{\partial^2}{\partial x_2^2} + V(x_1) + V(x_2) + U(x_1, x_2) , \quad (23)$$

where $U(x_1, x_2)$ is the potential energy due to the interaction between particles. We start from the so-called *non-interacting limit*, where we put $U(x_1, x_2) = 0$.

How do we construct the two-particle wave functions? The immediate idea is: given a complete set of single-particle states $\psi_l(x)$ indexed by a quantum number l , two-particle states should be indexed by a *pair* of quantum numbers, l_1 and l_2 , one for each particle. Thus, we can take as a basis set of two-body wave functions the products of the form

$$\psi_{l_1}(x_1)\psi_{l_2}(x_2) . \quad (24)$$

In a human language: “we put one particle into the state l_1 , and the other one into the state l_2 ”. Since particles do not interact with each other, the associated energy is just a sum $E_{l_1} + E_{l_2}$.

We now incorporate a basic principle of quantum mechanics, which states that *identical particles are indistinguishable from each other*. This means that observables cannot be changed by an interchange $x_1 \leftrightarrow x_2$. In particular, it means that the probability density of finding one particle at x_1 and another one at x_2 is invariant with respect to $x_1 \leftrightarrow x_2$:

$$|\Psi(x_1, x_2)|^2 = |\Psi(x_2, x_1)|^2 . \quad (25)$$

Therefore, the wave function itself must satisfy

$$\Psi(x_1, x_2) = \pm \Psi(x_2, x_1) . \quad (26)$$

Particles which require the plus sign in (26) are called *bosons*, and particles which require the minus sign are called *fermions*.²

²Technically, it is legitimate to consider more complicated objects, where the wave function acquires a complex phase under the particle interchange, i.e. $\Psi(x_1, x_2) = e^{i\phi} \Psi(x_2, x_1)$. Such objects are called *anyons*, and play a prominent role in certain theories. During this course we unfortunately do not have time to discuss any of these advanced topics in any detail.

Using (26) we amend (24) by constructing symmetric and antisymmetric wave functions

$$\Psi_{l_1, l_2}(x_1, x_2) = \mathcal{N}_b [\psi_{l_1}(x_1)\psi_{l_2}(x_2) + \psi_{l_1}(x_2)\psi_{l_2}(x_1)] \quad (\text{bosons}) , \quad (27)$$

and

$$\Psi_{l_1, l_2}(x_1, x_2) = \mathcal{N}_f [\psi_{l_1}(x_1)\psi_{l_2}(x_2) - \psi_{l_1}(x_2)\psi_{l_2}(x_1)] \quad (\text{fermions}) . \quad (28)$$

Here $\mathcal{N}_{b,f}$ are (yet undefined) normalization constants.

The symmetry requirements, Eq. (26), has profound consequences, some hints of which are already seen in Eqs. (27) and (28). Loosely speaking, bosons tend to bunch together, while fermions, on the contrary, don't like to be close to each other: the wave function (28) is zero for $x_1 = x_2$. Moreover—and more importantly—fermions cannot occupy the same quantum state: the wave function (28) is zero for all x_1 and x_2 if $l_1 = l_2$. (This is known as the Pauli exclusion principle.)

We now proceed to normalizing the wave functions (27) and (28). It is convenient to deal with bosons and fermions separately.

Bosons.— If both particles are in the same state, $l_1 = l_2 = l$, then Eq. (27) becomes $\Psi_{l,l}(1, 2) = \mathcal{N}_b \psi_l(x_1)\psi_l(x_2)$. Substituting this into (22), and using the orthonormality of the single-particle basis, Eq. (18), we find $\mathcal{N}_b = 1$.

Exercise 2 Now assume that $l_1 \neq l_2$. Show that in this case $\mathcal{N}_b = 1/\sqrt{2}$. Write out the resulting form of the wave function (27).

Exercise 3 Normalize the fermionic wave function (28). Notice that due to the Pauli exclusion principle the quantum numbers in (28) are necessarily different.

A final note is in order here. In fact, it turns out that particles with half-integer spin are fermions, while particles with integer spin are bosons. For example: electrons, neutrons and protons all have spin $1/2$, and are thus fermions. Statistics of composite particles is determined by the number of fermions it is made of: for example, the ^3He isotope consists of two protons and one neutron, and is a fermion. On the other hand, the ^4He isotope, made of two protons and two neutrons, is bosonic.

4 Many particles

In this section we will construct the wave functions for N identical particles. Just as in Sec. 3, a complete set of single-particle states, $\psi_l(x)$, generates a basis set for N -body functions as products of the form $\psi_{l_1}(x_1)\psi_{l_2}(x_2) \cdots \psi_{l_N}(x_N)$. A general form an N -body wave function can be written out in terms of this set:

$$\Psi(x_1, \dots, x_N) = \sum_{l_1, l_2, \dots, l_N} C(l_1, l_2, \dots, l_N) \psi_{l_1}(x_1)\psi_{l_2}(x_2) \cdots \psi_{l_N}(x_N) . \quad (29)$$

Indistinguishability of identical particles now requires that the wave function (29) is symmetric (for bosons) or antisymmetric (for fermions) under an exchange of any two particles, $x_i \leftrightarrow x_k$. Since under such an exchange the term of the form

$$C(\cdots, l_i, \cdots, l_k, \cdots) \cdots \psi_{l_i}(x_i) \cdots \psi_{l_k}(x_k) \cdots \quad (30)$$

becomes

$$C(\cdots, l_i, \cdots, l_k, \cdots) \cdots \psi_{l_i}(x_k) \cdots \psi_{l_k}(x_i) \cdots , \quad (31)$$

we see that the coefficients C in (29) must obey

$$C(\cdots, l_i, \cdots, l_k, \cdots) = \pm C(\cdots, l_k, \cdots, l_i, \cdots) \quad (32)$$

where bosons require the plus sign and fermions require the minus sign.

From now on we will deal with bosons and fermions separately. And we start with bosons.

4.1 Bosons

We now note that every quantum number l_i in the sum runs over the same set of integers. Since $C(l_1, \dots, l_N)$ is symmetric under exchanges of its arguments, we may group equal values of quantum numbers, while keeping track of how many times each value appears. Suppose that the value 1 appears n_1 times, the value 2 appears n_2 times, and so on. For example,

$$C(122311 \dots) = C(\underbrace{111 \dots}_{n_1 \text{ times}}, \underbrace{22 \dots}_{n_2 \text{ times}}, \dots) . \quad (33)$$

Notice that all the terms in (29) where the state 1 appears n_1 times, the state 2 appears n_2 times and so on, *all appear with the same coefficient in the sum*. We thus give this coefficient a new name:

$$\bar{C}(n_1, n_2, \dots, n_\infty) \equiv C(\underbrace{111 \dots}_{n_1}, \underbrace{22 \dots}_{n_2}, \dots) . \quad (34)$$

This way, we have just defined the so-called *occupation numbers*. This notion is, in fact, crucial for all the many-body theory(-ies).

We now proceed to normalization of the many-body wave function (29). Since the single-particle states are orthonormal, the normalization condition for the N -body wave function (29) reads

$$\sum_{l_1, l_2, \dots, l_N} |C(l_1, l_2, \dots, l_N)|^2 = 1 . \quad (35)$$

We now use the equality of the coefficients C with the same set of occupation numbers, and regroup the terms in the sum as follows:

$$\sum_{n_1, n_2, \dots, n_\infty} |\bar{C}(n_1, \dots, n_\infty)|^2 \sum_{\{l\} \text{ s.t. } \{n\}} 1 = 1 , \quad (36)$$

where the summation proceeds in two steps: first, we sum over all combinations of occupation numbers, and then over all combinations of quantum numbers $\{l\}$ consistent with a given set of occupation numbers $\{n\}$.

The second sum is easy to evaluate: we are essentially putting N objects (here: particles) into the boxes (here: single-particle states), so that there are n_1 objects in the 1st box, n_2 objects in the 2nd box, and so forth. The number of ways objects can be distributed over the boxes equals $N!/n_1!n_2! \dots n_\infty!$, therefore Eq. (36) becomes

$$\sum_{n_1, n_2, \dots, n_\infty} |\bar{C}(n_1, \dots, n_\infty)|^2 \frac{N!}{n_1!n_2! \dots n_\infty!} = 1 . \quad (37)$$

Notice that most n -s are zero, since the total is finite,

$$\sum_{i=1}^{\infty} n_i = N . \quad (38)$$

To simplify the notation, we introduce yet another coefficient,

$$f(n_1, \dots, n_\infty) = \bar{C}(n_1, \dots, n_\infty) \left(\frac{N!}{n_1!n_2! \dots n_\infty!} \right)^{1/2} , \quad (39)$$

which obeys

$$\sum_{n_1, \dots, n_\infty} |f(n_1, \dots, n_\infty)|^2 = 1 . \quad (40)$$

Finally, we can rewrite the wave function (29) in the form

$$\Psi(x_1, \dots, x_N) = \sum_{n_1, \dots, n_\infty} f(n_1, \dots, n_\infty) \Phi_{n_1, \dots, n_\infty}(x_1, \dots, x_N) , \quad (41)$$

where the summation *only* runs over the occupation numbers [which are only constrained by (38)], and

$$\Phi_{n_1, \dots, n_\infty}(x_1, \dots, x_N) = \left(\frac{n_1! n_2! \dots n_\infty!}{N!} \right)^{1/2} \sum_{\substack{\{l\} \\ \text{s.t. } \{n\}}} \psi_{l_1}(x_1) \psi_{l_2}(x_2) \dots \psi_{l_N}(x_N), \quad (42)$$

are the completely symmetrized orthonormal N -body basis functions. The summation in (42) is over all possible combinations of quantum numbers l_1, \dots, l_N consistent with a given set of occupation numbers n_1, \dots, n_∞ , exactly as in Eq. (36).

Exercise 4 Verify that for two bosons Eq. (42) reduces to (27).

Exercise 5 Write out the explicit form of the wave function (42) for three bosons, where two of them occupy the state 1, and the third one is in the state 2. Do not specify the form of the single-particle states.

4.2 Fermions

For fermions, the wave function (29) is antisymmetric under an exchange of any two particles, hence the coefficients C obey (32) with the minus sign.

First of all, we note that the Pauli exclusion principle prescribes that in the set of quantum numbers l_1, \dots, l_N in (29) *no two numbers can be equal to each other*: indeed, if in (32) $l_i = l_k$, then the only option is that $C(\dots, l_i, \dots, l_k, \dots) = 0$. Therefore, the Pauli exclusion principle can be states as follows:

$$\text{For fermions, occupation numbers can only be equal to zero or one.} \quad (43)$$

In order to fix the global sign, it is convenient to order the single-particle states, so that $l_1 < l_2 < \dots < l_N$. Since all coefficients in (29) which have the same states occupied are equal up to a minus sign, and we can define the coefficient \bar{C} via

$$\bar{C}(n_1, \dots, n_\infty) \equiv C(l_1 < l_2 < \dots < l_N). \quad (44)$$

Precisely as in the case of bosons, the wave function (29) can be expanded into

$$\Psi(x_1, \dots, x_N) = \sum_{n_1, \dots, n_\infty} f(n_1, \dots, n_\infty) \Phi_{n_1, \dots, n_\infty}(x_1, \dots, x_N), \quad (45)$$

where each occupation number can be either zero or one, and the basis functions now take the form of the so-called Slater determinants:

$$\Phi_{n_1, \dots, n_\infty}(x_1, \dots, x_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \psi_{l_1}(x_1) & \psi_{l_1}(x_2) & \dots & \psi_{l_1}(x_N) \\ \psi_{l_2}(x_1) & \psi_{l_2}(x_2) & \dots & \psi_{l_2}(x_N) \\ \vdots & \vdots & \ddots & \vdots \\ \psi_{l_N}(x_1) & \psi_{l_N}(x_2) & \dots & \psi_{l_N}(x_N) \end{vmatrix}. \quad (46)$$

Notice the structure of the Slater determinant: in each row the quantum numbers are the same, while in each column the coordinates are the same.

Exchanging two coordinates of two particles means exchanging two columns of a determinant, which brings in a minus sign, as required by fermionic nature of the wave functions. Furthermore, having two quantum numbers equal to each other means that the determinant has two rows equal to each other, and is thus equal zero.

Exercise 6 Write out the Slater determinant explicitly for $N = 2$. Compare to Eq. (28)

5 Second quantization

In the previous section we worked out the wave functions for N bosons or fermions. Working with these functions directly is extremely inconvenient. In this section we develop a more convenient formalism—the so-called *second quantization* formalism.

We start by looking at the kinetic energy operator, which is nothing but a sum of kinetic energies of each individual particles

$$\hat{T} = \sum_{a=1}^N \hat{T}_a , \quad (47)$$

where from now on we use the index a to label the *particles*. Each of the operators \hat{T}_a only acts on the coordinates of the particle a , and is explicitly given by $\hat{T}_a = -\hbar^2/2m \partial^2/\partial x_a^2$.

Taking as the set of single-particle states the eigenstates of the kinetic energy operator, we have

$$\hat{T}_a \psi_k(x_a) = \epsilon_k \psi_k(x_a) , \quad (48)$$

where we label the single particle states by an index k (which we do from now on). Therefore, acting by \hat{T}_a onto the now-familiar product of single-particle states, we have

$$\hat{T}_a \psi_{k_1}(x_1) \cdots \psi_{k_a}(x_a) \cdots \psi_{k_N}(x_N) = \epsilon_{k_a} \psi_{k_1}(x_1) \cdots \psi_{k_a}(x_a) \cdots \psi_{k_N}(x_N) . \quad (49)$$

Combining this result with (47), we find

$$\hat{T} \psi_{k_1}(x_1) \cdots \psi_{k_a}(x_a) \cdots \psi_{k_N}(x_N) = \left(\sum_{a=1}^N \epsilon_{k_a} \right) \psi_{k_1}(x_1) \cdots \psi_{k_a}(x_a) \cdots \psi_{k_N}(x_N) . \quad (50)$$

Now let's take a closer look at the bracketed sum in this formula. Here the summation runs over the particles in the system, and k_a are the quantum numbers. We have already introduced occupation numbers n_k which count how many particles are in a state k . Therefore—and it is the *crucial point of the whole derivation*—we can convert the sum over particles, $\sum_{a=1}^N \epsilon_{k_a}$ into the sum over the single-particle states, $\sum_k n_k \epsilon_k$. Recalling that both bosonic (42) and fermionic (46) N -body wave functions are nothing but appropriate linear combinations of the products of the single-particle states, we find

$$\hat{T} \Phi_{n_1, \dots, n_\infty}(x_1, \dots, x_N) = \left(\sum_k n_k \epsilon_k \right) \Phi_{n_1, \dots, n_\infty}(x_1, \dots, x_N) . \quad (51)$$

Notice that the sum in brackets here is nothing but a total kinetic energy of N particles, written in the occupation number representation.

Introducing the Dirac bra/ket notation $|n_1, \dots, n_\infty\rangle$ for $\Phi_{n_1, \dots, n_\infty}(x_1, \dots, x_N)$, we can rewrite Eq. (51) in a more compact form

$$\langle n_1, \dots, n_\infty | \hat{T} | n_1, \dots, n_\infty \rangle = \sum_k n_k \epsilon_k , \quad (52)$$

which literally says: “the diagonal matrix element of the kinetic energy equals the sum over all the single-particle states of the kinetic energy of a particle in that state times the occupation number of the state”.

Notice that the only difference between bosons and fermions at this point is that for bosons the occupation numbers can take any value, $n_k = 0, 1, 2, \dots$, while for fermions $n_k = 0$ or 1 only.

In fact, such construction is not limited to the kinetic energy operator. For *any* one-body operator,

$$\hat{O} = \sum_{a=1}^N \hat{O}_a^{(1)} , \quad (53)$$

we simply repeat the steps (47) to (52) and arrive at

$$\langle n_1, \dots, n_\infty | \hat{\mathcal{O}} | n_1, \dots, n_\infty \rangle = \sum_k n_k \langle \psi_k | \hat{\mathcal{O}}^{(1)} | \psi_k \rangle , \quad (54)$$

where we have also introduced the Dirac notation for the single-particle matrix elements. Notice that in writing the latter matrix elements, we do not need to specify which particle does the operator belong to. In other words, instead of dealing with N -dimensional functions [cf the lhs of (54)] we only have to work with single-particle objects [cf the rhs of (54)].

As an example, we work out the matrix elements of the density operator $\hat{\rho}(x)$:

$$\hat{\rho}(x) = \sum_{a=1}^N \delta(x - x_a) , \quad (55)$$

where $\delta(x)$ is the Dirac δ -function: $\delta(x \neq 0) = 0$, and $\delta(x \rightarrow 0) \rightarrow \infty$ such that

$$\int_{-\infty}^{\infty} \delta(x) dx = 1 ,$$

and for any function $f(x)$ which is continuous at $x \rightarrow 0$

$$\int_{-\infty}^{\infty} f(x) \delta(x) dx = f(0) .$$

Working out the matrix elements of $\hat{\rho}(x)$ using the wave functions (42) or (46) looks formidable, but using (54) is easy:

$$\langle \psi_k | \delta(x - x_a) | \psi_k \rangle \equiv \int dx_a \psi_k^*(x_a) \delta(x - x_a) \psi_k(x_a) = |\psi_k(x)|^2 , \quad (56)$$

and therefore

$$\langle n_1, \dots, n_\infty | \hat{\rho}(x) | n_1, \dots, n_\infty \rangle = \sum_k n_k |\psi_k(x)|^2 . \quad (57)$$

Exercise 7 Using (54), calculate the diagonal matrix elements of the momentum operator, taking as the single-particle basis the states you've constructed in Assignment 1. Interpret your results.

It is worth reiterating that the results (52), (54) and (57) are valid for both bosons and fermions, the only difference being that fermionic occupation numbers are 0 or 1, while bosonic occupation numbers are free from this restriction.

Once we consider *off-diagonal* matrix elements of one-body operators, bosons and fermions start being significantly different and it is convenient to consider them separately.

5.1 Bosons

Consider a situation where a particle collides with a stationary obstacle. In course of a collision, the particle is deflected, hence its momentum changes from \mathbf{p} to \mathbf{p}' . In quantum mechanics we say that without an obstacle the momentum is a good quantum number, hence the wave function of a particle can be taken just as a plane wave, $|\mathbf{p}\rangle$, while in presence of an obstacle the momentum is no longer conserved. The interaction of a particle with an obstacle is described by a matrix element $\langle \mathbf{p}' | \hat{V} | \mathbf{p} \rangle$, where $\hat{V} = V(\mathbf{r} - \mathbf{R})$ is an interaction potential between a particle at point \mathbf{r} and an obstacle at point \mathbf{R} .



Now, consider a system of N particles in presence of an obstacle. To account for an effect of an obstacle we need to take into account the fact all the particles can now scatter off it, hence the operator describing it will be

$$\hat{V} = \sum_{a=1}^N V(\mathbf{r}_a - \mathbf{R}) , \quad (58)$$

which has the general form of a one-body operator (53), and the scattering is described by its matrix elements between states with differing sets of occupation numbers: as compared to the initial state, the final state has an extra particle with momentum $|\mathbf{p}'\rangle$ and one less particle with momentum $|\mathbf{p}\rangle$. Calculating such matrix elements is straightforward but rather tedious.

We will not do the full calculation here, we will only state the result, which can be written in a rather compact form if we use the Dirac notation for the occupation number states. Assuming that the single-particle state $|\mathbf{p}\rangle$ has number k and the state $|\mathbf{p}'\rangle$ has number i , we have that the only non-zero matrix elements of the operator (53) are

$$\langle \dots, n_i + 1, \dots, n_k - 1, \dots | \hat{\mathcal{O}} | \dots, n_i, \dots, n_k, \dots \rangle = \langle \psi_i | \hat{\mathcal{O}}^{(1)} | \psi_k \rangle \sqrt{(n_i + 1)n_k} . \quad (59)$$

Technically, Eqs. (54) and (59) completely define the matrix structure of one-body operators (53) in the space of the occupation numbers. Nevertheless, the notation is still a somewhat clumsy, and it is convenient to reformulate the formalism a little further.

5.1.1 Creation and annihilation operators (Bosons.)

For clarity, we start by focusing on one particular single-particle state, say, a state number k . For state k , we define the so-called *annihilation operator* such that

$$\hat{b}_k |n_k\rangle = \sqrt{n_k} |n_k - 1\rangle . \quad (60)$$

Just as its name implies, acting on a state with occupation number n_k , this operator generates a state with one less particle. The annihilation operator is *not* hermitian: its hermitian conjugate is

$$\hat{b}_k^\dagger |n_k\rangle = \sqrt{n_k + 1} |n_k + 1\rangle , \quad (61)$$

and it is universally known as a *creation operator*.

Consider acting on the state $|n_k\rangle$ by both creation and annihilation operators sequentially:

$$\hat{b}_k^\dagger \hat{b}_k |n_k\rangle = \hat{b}_k^\dagger \sqrt{n_k} |n_k - 1\rangle = n_k |n_k\rangle , \quad (62)$$

$$\hat{b}_k \hat{b}_k^\dagger |n_k\rangle = \hat{b}_k \sqrt{n_k + 1} |n_k + 1\rangle = (n_k + 1) |n_k\rangle , \quad (63)$$

so that *creation and annihilation operators do not commute with each other*. Their commutator is

$$[\hat{b}_k, \hat{b}_k^\dagger] \equiv \hat{b}_k \hat{b}_k^\dagger - \hat{b}_k^\dagger \hat{b}_k = 1 . \quad (64)$$

At this point you probably recognize that you've already met these operators before— when discussing the harmonic oscillator.

In the present context we have a whole collection of single-particle states, $k = 1, 2, \dots$, hence we define the creation and annihilation operators for each of these. Since, by assumption, the single-particle states are labeled by good quantum numbers, different states are independent, and we require that creation and annihilation operators for different states commute with each other:

$$[\hat{b}_i, \hat{b}_k] = 0 \quad (65)$$

$$[\hat{b}_i, \hat{b}_k^\dagger] = \delta_{ik} . \quad (66)$$

At this point we note in passing that, in fact, *all* the properties of creation and annihilation operators can be derived exclusively from the commutation relations (65) and (66).

Looking at Eq. (62) we see that the operator $\hat{b}_k^\dagger \hat{b}_k$ acts as counting operator— it is diagonal in the occupation number basis, and its eigenvalues are just occupation numbers themselves. It is customary to denote it as $\hat{n}_k = \hat{b}_k^\dagger \hat{b}_k$, so that

$$\hat{n}_k |n_k\rangle = n_k |n_k\rangle . \quad (67)$$

Now compare (67) to (57). We see that we reproduce the matrix elements (57) by identifying

$$\hat{\rho}(x) = \sum_k |\psi_k(x)|^2 \hat{n}_k . \quad (68)$$

In view of this connection, the counting operator \hat{n}_k is nothing but *density operator in the second quantized representation*.

Moreover, for any one-body operator (53) we reproduce the matrix elements (54) and (59) by identifying

$$\hat{O} = \sum_{ik} \hat{b}_i^\dagger \langle \psi_i | \hat{O}^{(1)} | \psi_k \rangle \hat{b}_k . \quad (69)$$

Notice that here all the summation is performed over the single-particle *states*, and individual particles' coordinates do not appear *at all*.

The result (69) is remarkable: in the first-quantized form, we have an N -dimensional operator acting on rather complicated functions of N variables (42); in the second-quantized form, (69), we have to calculate one-dimensional matrix elements only. The rest is automatically taken care of by the algebra of creation and annihilation operators.

Exercise 8 Establish the commutation relation $[\hat{n}_i, \hat{b}_k]$. *Hint: This can be done by either a direct calculation similar to (62) or by using the commutation relations (65).*

Exercise 9 Establish the commutation relation $[\hat{n}_i, \hat{n}_k]$. *Hint: Results of the previous problem come in handy.*

Exercise 10 Write down the second-quantized form of the momentum operator. Compare to Assignment 7.

Exercise 11 Given a Hamiltonian in the form

$$\hat{H} = \sum_k \epsilon_k \hat{b}_k^\dagger \hat{b}_k ,$$

establish the commutation relations $[\hat{H}, \hat{b}_k]$ and $[\hat{H}, \hat{b}_k^\dagger]$.

As an example of the algebra of creation and annihilation operators we work out an explicit construction of the basis states in the occupation number space. We start from a state $|n_k\rangle$ and apply (60) repeatedly:

$$\begin{aligned} \hat{b}_k |n_k\rangle &= \sqrt{n_k} |n_k - 1\rangle , \\ \hat{b}_k |n_k - 1\rangle &= \sqrt{n_k - 1} |n_k - 2\rangle , \\ &\vdots \\ \hat{b}_k |1_k\rangle &= 1 |0_k\rangle , \\ \hat{b}_k |0_k\rangle &= 0 . \end{aligned} \quad (70)$$

Since an occupation number cannot be negative, by reducing the number of particles in the state k , we eventually arrive at the stage where it is empty, which we denote by $|0_k\rangle$. Acting on this state with an annihilation operator again, we are bound to have a zero eigenvalue, i.e. the last line of (70). We typically call such situation a *vacuum*. Now, starting from a vacuum state and applying the creation operator repeatedly, we find

$$|n_k\rangle = \frac{1}{\sqrt{n_k!}} (\hat{b}_k^\dagger)^{n_k} |0_k\rangle . \quad (71)$$

Two-body operators So far we have only dealt with one-body operators of the form (53). Another important class of operators are *two-body* operators, e.g. interaction between particles. A general form of a two-body operator is

$$\hat{U} = \sum_{a>b} \hat{U}_{a,b}^{(2)}, \quad (72)$$

where the sum runs over all pairs of particles in the system. A second-quantized form of two-body operators can be established just in the same way as for the one-body operators. The result is

$$\hat{U} = \frac{1}{2} \sum_{rstu} \hat{b}_r^\dagger \hat{b}_s^\dagger \langle rs | \hat{U}^{(2)} | tu \rangle \hat{b}_t \hat{b}_u, \quad (73)$$

where r, s, t and u are single-particle *states*.

Exercise 12 Consider a gas where the interaction between particles is short-ranged and can be modeled by the so-called contact interaction

$$U(x_a - x_b) = g\delta(x_a - x_b),$$

where g is some constant. Write down a second-quantized form for the operator of the total interaction energy.

5.2 Creation and annihilation operators (Fermions.)

Dealing with fermionic particles is at the same time both easier and more complicated than dealing with bosons at. It is easier because the fermionic occupation numbers can only take values zero and one, so that the Hilbert space of occupation numbers for a single mode k only consists of two states, $|0_k\rangle$ and $|1_k\rangle$. It is more complicated because for antisymmetric wave functions (46) it is requisite to keep track of *signs*. This is rather messy in first quantization, but can be completely accounted for in the second quantization if we define the fermionic creation and annihilation operators via the *anticommutation* relations

$$\begin{aligned} \{\hat{c}_i, \hat{c}_k^\dagger\} &= \delta_{ik}, \\ \{\hat{c}_i, \hat{c}_k\} &= 0, \end{aligned} \quad (74)$$

where an $\{A, B\} = AB + BA$ is an *anticommutator*. From these relation it is easy to check that $\hat{c}_k^2 = 0$, which is one more guise of the Pauli exclusion principle.

As an example of the fermionic algebra we define the number operator $\hat{n}_k = \hat{c}_k^\dagger \hat{c}_k$ and work out what is \hat{n}_k^2 (dropping the subscript to lighten the notation):

$$\hat{n}_k^2 = (1 - \hat{c} \hat{c}^\dagger)^2 \quad \text{using (74)} \quad (75)$$

$$= 1 - 2\hat{c} \hat{c}^\dagger + \hat{c} \hat{c}^\dagger \hat{c} \hat{c}^\dagger \quad (76)$$

$$= 1 - 2\hat{c} \hat{c}^\dagger + \hat{c}(1 - \hat{c} \hat{c}^\dagger)\hat{c}^\dagger \quad \text{using (74)} \quad (77)$$

$$= 1 - \hat{c} \hat{c}^\dagger \quad \text{using the Pauli principle} \quad (78)$$

$$= \hat{n}_k. \quad (79)$$

From this we see once more that the the eigenvalues of \hat{n} can be only 0 and 1.

Exercise 13 Check that the number operators for different modes commute with each other, so that $[\hat{n}_i, \hat{n}_k] = 0$.

The action of the fermionic operators onto the occupation numbers basis states is simple in case of a single mode:

$$\begin{aligned}\hat{c}^\dagger |0\rangle &= |1\rangle & \hat{c} |0\rangle &= 0 , \\ \hat{c}^\dagger |1\rangle &= 0 & \hat{c} |1\rangle &= |0\rangle ,\end{aligned}\tag{80}$$

so that not only the annihilation operator annihilates the vacuum, but also the creation operator annihilates $|1\rangle$.

The occupation number basis states $|n_1, \dots, n_\infty\rangle$ can be constructed explicitly as cartesian products of the single-particle states in a way similar to that of bosons:

$$|n_1, \dots, n_\infty\rangle = \left(\hat{c}_1^\dagger\right)^{n_1} \left(\hat{c}_2^\dagger\right)^{n_2} \dots \left(\hat{c}_\infty^\dagger\right)^{n_\infty} |0\rangle ,\tag{81}$$

but the action of the operators onto these states is a little more complicated than in the bosonic case. Indeed, acting on this state by \hat{c}_k we find

$$\hat{c}_k |n_1, n_2, \dots, n_k, \dots, n_\infty\rangle = (-)^{S_k} \left(\hat{c}_1^\dagger\right)^{n_1} \left(\hat{c}_2^\dagger\right)^{n_2} \dots \hat{c}_k \left(\hat{c}_k^\dagger\right)^{n_k} \dots \left(\hat{c}_\infty^\dagger\right)^{n_\infty} |0\rangle ,\tag{82}$$

where

$$S_k = n_1 + n_2 + \dots + n_{k-1} .\tag{83}$$

The factor $(-)^{S_k}$ arises from the fact that we use the commutation relations (74) $k-1$ times to move \hat{c}_k towards \hat{c}_k^\dagger . Now, if $n_k = 0$, then we may move \hat{c}_k all the way towards the vacuum, where it gives zero in accordance with (80). If, on the other hand, $n_k = 1$, then we write $\hat{c}_k \hat{c}_k^\dagger = 1 - \hat{c}_k^\dagger \hat{c}_k$, and in the second term again move the annihilation operator all the way to the vacuum, so that the second term disappears. The first term which remains, has the form (81) with $n_k = 0$.

This way, we find

$$\hat{c}_k |\dots, 1_k, \dots\rangle = (-)^{S_k} |\dots, 0_k, \dots\rangle \qquad \hat{c}_k |\dots, 0_k, \dots\rangle = 0 ,\tag{84}$$

$$\hat{c}_k^\dagger |\dots, 0_k, \dots\rangle = (-)^{S_k} |\dots, 1_k, \dots\rangle \qquad \hat{c}_k^\dagger |\dots, 1_k, \dots\rangle = 0 ,\tag{85}$$

$$\hat{n}_k |\dots, n_k, \dots\rangle = n_k |\dots, n_k, \dots\rangle .\tag{86}$$

Here S_k is given by (83) and we see that for the number operator the phase factors cancel.

A direct if messy calculation shows that the phase factors in (86) exactly correspond to the signs due to permutations in Slater determinants (46), so that the second quantized form of both one-body and two-body operators, Eq. (53) and (72) is similar to the bosonic case, with \hat{c} -s instead of \hat{b} -s:

$$\hat{\mathcal{O}} = \sum_{ik} \hat{c}_i^\dagger \langle \psi_i | \hat{\mathcal{O}}^{(1)} | \psi_k \rangle \hat{c}_k ,\tag{87}$$

and

$$\hat{\mathcal{U}} = \frac{1}{2} \sum_{rstu} \hat{c}_r^\dagger \hat{c}_s^\dagger \langle rs | \hat{\mathcal{U}}^{(2)} | tu \rangle \hat{c}_t \hat{c}_u .\tag{88}$$

Exercise 14 Given a Hamiltonian in the form

$$\hat{H} = \sum_k \epsilon_k \hat{c}_k^\dagger \hat{c}_k ,$$

establish the commutation relations $[\hat{H}, \hat{c}_k]$ and $[\hat{H}, \hat{c}_k^\dagger]$.

5.3 Field operators

We are going to reformulate the formalism a little further yet. We define the so-called *field operators*,

$$\begin{aligned}\hat{\psi}(x) &= \sum_k \psi_k(x) \hat{b}_k && (\text{bosons}) , \\ \hat{\psi}(x) &= \sum_k \psi_k(x) \hat{c}_k && (\text{fermions}) .\end{aligned}\tag{89}$$

We stress that these objects are *not* wave functions, these are operators which act on the elements of the Hilbert space of occupation number states.

Using the field operators the second-quantized form of the particle number operator takes the form

$$\hat{N} = \int \hat{\psi}^\dagger(x) \hat{\psi}(x) dx .\tag{90}$$

Indeed, substituting (89) into the definition (90) and using the orthonormality of the single-particle basis, (18), we find $\hat{N} = \sum_k \hat{n}_k$. Acting with such operator on a state $|n_1, \dots, n_\infty\rangle$ yields the sum of the occupation numbers of all the states, which is nothing but the total number of particles in the system.

Exercise 15 *Prove that (90) is indeed diagonal in the occupation state basis, $|n_1, n_2, \dots, n_\infty\rangle$, and that it's eigenvalues are the total number of particles.*

Given the total particle number operator (90), we identify the density operator (55)

$$\hat{\rho}(x) = \hat{\psi}^\dagger(x) \hat{\psi}(x) .\tag{91}$$

The commutation relations for the field operators follow directly from the commutation relations for the creation and annihilation operators. In particular:

$$\begin{array}{ll} \text{bosons} & \text{fermions} \\ \left[\hat{\psi}(x), \hat{\psi}^\dagger(y) \right] = \delta(x - y) & \left\{ \hat{\psi}(x), \hat{\psi}^\dagger(y) \right\} = \delta(x - y) \end{array}\tag{92}$$

$$\begin{array}{ll} \left[\hat{\psi}(x), \hat{\psi}(y) \right] = 0 & \left\{ \hat{\psi}(x), \hat{\psi}(y) \right\} = 0 \end{array}\tag{93}$$

As an example, we prove the bosonic version of (92): Using (89) we find

$$\hat{\psi}(x) \hat{\psi}^\dagger(y) = \sum_{k, k'} \psi_k(x) \psi_{k'}^*(y) \hat{b}_k \hat{b}_{k'}^\dagger\tag{94}$$

$$\hat{\psi}^\dagger(y) \hat{\psi}(x) = \sum_{k, k'} \psi_k(x) \psi_{k'}^*(y) \hat{b}_{k'}^\dagger \hat{b}_k ,\tag{95}$$

and therefore

$$\left[\hat{\psi}(x), \hat{\psi}^\dagger(y) \right] = \sum_{k, k'} \psi_k(x) \psi_{k'}^*(y) \left[\hat{b}_k, \hat{b}_{k'}^\dagger \right] \quad \text{using (66)}\tag{96}$$

$$= \sum_k \psi_k(x) \psi_k^*(y)\tag{97}$$

$$= \delta(x - y) ,\tag{98}$$

where in the last line we used the completeness of the set of the single-particle states $\{\psi_k(x)\}$,

$$\sum_k \psi_k(x) \psi_k^*(y) = \delta(x - y) .\tag{99}$$

Proving the other relations in (92) and (93) is similar.

Exercise 16 *Prove the fermionic version of (93).*

Exercise 17 *Calculate the commutator $[\hat{\psi}(x), \hat{N}]$ for bosonic fields.*

Exercise 18 *Calculate the commutator $[\hat{\psi}(x), \hat{N}]$ for fermionic fields.*

Using the field operators we can write the second-quantized form of the one- and two-body operators, (53) and (72), in the following form:

$$\hat{O} = \int \hat{\psi}^\dagger(x) \hat{O}^{(1)}(x) \hat{\psi}(x) dx , \quad (100)$$

and

$$\hat{U} = \frac{1}{2} \iint \hat{\psi}^\dagger(x) \hat{\psi}^\dagger(y) \hat{U}^{(2)}(x, y) \hat{\psi}(y) \hat{\psi}(x) dx dy . \quad (101)$$

Notice the order of the arguments of the ψ -operators in the expression for a two-body operator. This is especially important in fermionic case, because the fermionic operators anticommute, and a typo at this level may lead to an overall sign change.

Exercise 19 *Given a gas of N identical bosons with a Hamiltonian in first quantization*

$$\hat{H} = \sum_{a=1}^N \frac{\hat{\mathbf{p}}_a^2}{2m} + \sum_{a>b} V(\mathbf{r}_a - \mathbf{r}_b) , \quad (102)$$

write down the second-quantized form of the Hamiltonian

- *using the creation and annihilation operators;*
- *using the field operators.*

Exercise 20 *Repeat the previous assignment for N identical fermions.*

Exercise 21 *On physical grounds, we expect that the Hamiltonian (102) does not change the number of particles. Check that, indeed, the total number of particles, (90), commutes with the Hamiltonian (102).*

Exercise 22 *Consider a gas of N identical fermions, governed by a Hamiltonian (102). Using as the single-particle basis the solutions of Assignment 1, evaluate the interaction part of the Hamiltonian. The final result will contain the Fourier transform of the interaction potential.*

Exercise 23 *Consider a two-body operator (101) for bosonic fields. Using commutation relations (92), express (101) in terms of the density operator (91).*

Exercise 24 *Repeat the previous assignment for fermionic fields.*

6 Statistical mechanics of Bose and Fermi gases

Consider a gas in a thermal equilibrium at temperature T . In statistical mechanics we are interested in the properties of a gas in the so-called *thermodynamic limit*, where both number of particles $N \rightarrow \infty$ and the volume $V \rightarrow \infty$ such that the average density $n = N/V$ is finite.

There are multiple ways of taking such limit. In the so-called *canonical ensemble* we fix both N and V and take the limit at the end of a calculation. In the canonical ensemble, the probability of a system occupying a microscopic state ν with the energy E_ν is given by the *Gibbs distribution*

$$w_\nu \propto e^{-E_\nu/T} . \quad (103)$$

Notice that from now on we measure the temperature in energy units, so that $k_B = 1$. From the quantum mechanical point of view, the index ν in this equation labels the eigenstates of the Hamiltonian of the gas *at fixed number of particles*,

$$\hat{H} |\nu\rangle = E_\nu |\nu\rangle \quad (\text{fixed } N) . \quad (104)$$

Working with fixed N proves rather inconvenient, we will use the so-called *grand canonical ensemble*, where we allow the particle number to vary, but include a corresponding Lagrange multiplier to keep the mean value of $n = \langle N \rangle / V$ finite. This way, the Gibbs distribution takes the form

$$w_{N,\nu} = e^{(E_\nu^{(N)} - \mu N)/T} / Z \quad (\text{any } N) , \quad (105)$$

where $E_\nu^{(N)}$ is the energy of a state ν which has N particles, and μ is the so-called *chemical potential*. Here the normalization factor Z is known as the *grand partition function*, and is explicitly given by

$$Z = \sum_N \sum_\nu e^{-(E_\nu^{(N)} - \mu N)/T} . \quad (106)$$

Here at each N we sum over all states allowed at this number of particles. The grand canonical analog of the free energy is known as the *grand potential*,

$$\Omega(T, V, \mu) = -T \ln Z . \quad (107)$$

Quantum mechanically, we assume that the Hamiltonian conserves the particle number, so that the corresponding operators commute, $[\hat{H}, \hat{N}] = 0$, and thus both can be diagonalized simultaneously. That is,

$$\hat{H} |\nu; N\rangle = E_\nu^{(N)} |\nu; N\rangle , \quad (108)$$

$$\hat{N} |\nu; N\rangle = N |\nu; N\rangle . \quad (109)$$

This way, we see that (106) is nothing but the sum of the diagonal matrix elements of the operator $e^{-(\hat{H} - \mu \hat{N})/T}$. The sum of the diagonal elements of a matrix is known as its *trace*, and we write

$$Z = \text{Tr} e^{-(\hat{H} - \mu \hat{N})/T} . \quad (110)$$

This form of the partition function is particularly useful because the trace is invariant under the change of basis, i.e. Eq. (110) can be evaluated using any complete and orthonormal set of many-body states (for example: the basis of the occupation number states, constructed in the previous section.)

The notion of a partition function plays a major role in statistical physics because all the

thermodynamic potentials can be evaluated as its appropriate derivatives. For example,

$$\begin{aligned}
\frac{\partial}{\partial T} \ln Z &= \frac{1}{Z} \frac{\partial}{\partial T} \sum_{\nu, N} e^{-(E_\nu^{(N)} - \mu N)/T} \\
&= \frac{1}{Z} \sum_{\nu, N} \frac{(E_\nu^{(N)} - \mu N)}{T^2} e^{-(E_\nu^{(N)} - \mu N)/T} \\
&= \frac{1}{T^2} (\langle E \rangle - \mu \langle N \rangle) .
\end{aligned} \tag{111}$$

In writing the last line we used the angular brackets $\langle \dots \rangle$ for the thermal averages, so that by definition, the internal energy

$$\langle E \rangle \equiv \frac{\sum_{\nu, N} E_\nu^{(N)} e^{-(E_\nu^{(N)} - \mu N)/T}}{\sum_{\nu, N} e^{-(E_\nu^{(N)} - \mu N)/T}} , \tag{112}$$

and the average particle number

$$\begin{aligned}
\langle N \rangle &\equiv \frac{\sum_{\nu, N} N e^{-(E_\nu^{(N)} - \mu N)/T}}{\sum_{\nu, N} e^{-(E_\nu^{(N)} - \mu N)/T}} \\
&= T \frac{\partial}{\partial \mu} \ln Z .
\end{aligned} \tag{113}$$

At this point we make two observations. First, thermodynamic averages can be written as quantum mechanical traces. For example, Eq. (112) can be written as

$$\langle E \rangle = \frac{\text{Tr } \hat{H} e^{-(\hat{H} - \mu \hat{N})/T}}{\text{Tr } e^{-(\hat{H} - \mu \hat{N})/T}} . \tag{114}$$

Second, Eqs. (111), (112) and (113) give thermodynamic potentials *as functions of the chemical potential*. The connection to a more familiar canonic ensemble is then made as follows: calculate the partition function as a function μ and T , and then tune μ so that Eq. (113) yields the desired particle number.

6.1 Ideal gases

In this section we apply the formalism of statistical mechanics to the ideal Fermi and Bose gases. We assume that the gas is confined to box of a linear size L , so that the volume is $V = L^d$, where $d = 3$ is the dimensionality of space. It is convenient to use periodic boundary conditions in all three spatial dimensions, so that single-particle wavefunctions are the three-dimensional generalizations of the functions constructed in Assignment 1. Each single-particle state is then characterized by three momenta k_x, k_y and k_z , and, for spinful particles, the spin projection σ . For brevity, we denote the set of k_x, k_y, k_z and σ by a single letter k .

It is convenient to work in the occupation number representation, so that for the states $|\nu; N\rangle$ we take the occupation number states $|\{n_k\}\rangle$. In this representation, both Hamiltonian and particle number operators are diagonal [compare to Eq. (67)]:

$$\hat{H} = \sum_k \epsilon_k \hat{n}_k , \tag{115}$$

$$\hat{N} = \sum_k \hat{n}_k . \tag{116}$$

Therefore, in Eq. (110) we can replace the operators the c -numbers and arrive at

$$\begin{aligned}
Z &= \sum_{\{n_k\}} e^{-\beta \sum_k (\epsilon_k - \mu) n_k} \quad (\text{using } e^{a+b} = e^a e^b) \\
&= \sum_{\{n_k\}} \prod_k e^{-\beta (\epsilon_k - \mu) n_k} \\
&= \prod_k \sum_{n_k} e^{-\beta (\epsilon_k - \mu) n_k}, \tag{117}
\end{aligned}$$

where we also used a standard shorthand $\beta = 1/T$.

At this point we see a stark difference between bosons and fermions: Fermionic occupation numbers $n_k = 0, 1$ while bosonic occupation numbers $n_k = 0, 1, 2, \dots, \infty$. Therefore,

$$Z_{(\text{fermions})} = \prod_k \left(1 + e^{-\beta (\epsilon_k - \mu)} \right), \tag{118}$$

$$Z_{(\text{bosons})} = \prod_k \left(1 + e^{-\beta (\epsilon_k - \mu) \times 1} + e^{-\beta (\epsilon_k - \mu) \times 2} + \dots \right). \tag{119}$$

The sum in brackets in the second equation here is nothing but a geometric series,

$$1 + x + x^2 + \dots = \begin{cases} \frac{1}{1-x} & \text{if } |x| < 1, \\ \text{diverges} & \text{otherwise.} \end{cases}$$

Therefore, the series for the bosonic partition functions only converges if $\epsilon_k - \mu > 0$ for all states k , which sets the upper limit for the allowed values for the chemical potential, $\mu < \min_k \epsilon_k$. For $\epsilon_k = k^2/2m$, this implies $\mu < 0$. In this case, we have

$$Z_{(\text{bosons})} = \prod_k \frac{1}{1 - e^{-\beta (\epsilon_k - \mu)}}. \tag{120}$$

Using the definition of the grand potential, (107), we thus have

$$\Omega_{(\text{fermions})} = -T \sum_k \ln \left(1 + e^{-\beta (\epsilon_k - \mu)} \right), \tag{121}$$

$$\Omega_{(\text{bosons})} = +T \sum_k \ln \left(1 - e^{-\beta (\epsilon_k - \mu)} \right). \tag{122}$$

Using (113) and (107) we can now relate the chemical potential and particle number. For bosons we differentiate (122) with respect to μ and arrive at

$$\langle N \rangle = \sum_k \frac{1}{e^{\beta (\epsilon_k - \mu)} - 1}. \tag{123}$$

Since the rhs here involves the sum over the single-particle states, we write $\langle N \rangle = \sum_k \bar{n}_k$, where

$$\bar{n}_k = \frac{1}{e^{\beta (\epsilon_k - \mu)} - 1}, \tag{124}$$

is nothing but *an average value of the occupation number of the state k in thermal equilibrium*. The rhs of (124) is often referred to as the *Bose function*.

Exercise 25 Use (121), (113) and (107) to derive the analog of (124) for fermions. Comment on the differences to the bosonic case.

Having derived the equilibrium values of the occupation numbers, we can now immediately write down the average value of the energy in thermal equilibrium:

$$\langle E \rangle = \sum_k \epsilon_k \bar{n}_k, \tag{125}$$

where \bar{n}_k are given by Eq. (124) for bosons and by the solutions of the Assignment 25 for fermions.

6.2 The thermodynamic limit

Results of the previous section are, in fact, applicable to gases with finite number of particles confined to a finite volume. In this section we develop the formalism further under an assumption that containing volume of the gas is large.

We start from Eq. (123). The sum over k runs over the single-particle momenta \mathbf{k} (and spin projections for spinful particles). For simplicity we assume that single-particle energies do not depend on the spin projection—i.e. we assume that no magnetic field is applied. In this case, the summation over the spin variables for spin- s particles simply yields a multiplicative factor $g = 2s+1$. To evaluate the sum over momenta we recall the solution of the Assignment 1: $k_\alpha = 2\pi n_\alpha/L$, where $\alpha = x, y, z$ and $n_\alpha = 0, \pm 1, \pm 2, \dots$ (we put $\hbar = 1$ here). In the thermodynamic limit $L \rightarrow \infty$, and *the sum over momenta can be replaced by an integral* according to the prescription

$$\sum_{\mathbf{k}} (\dots) \longrightarrow V \int \frac{d^d \mathbf{k}}{(2\pi)^d} (\dots), \quad L \rightarrow \infty. \quad (126)$$

Indeed, the difference Δk_x between the consecutive momenta $k_x = 2\pi n_x/L$ and $k_x + \Delta k_x = 2\pi(n_x + \Delta n)/L$ where $\Delta n = 1$ tends to zero as $L \rightarrow \infty$, therefore,

$$\begin{aligned} \sum_{k_x} f(k_x) &\equiv \sum_{n_x=-\infty}^{\infty} f\left(\frac{2\pi n_x}{L}\right) \Delta n \quad (\Delta n = 1) \\ &= \frac{L}{2\pi} \sum_{n_x=-\infty}^{\infty} f\left(\frac{2\pi n_x}{L}\right) \Delta k_x \\ &\rightarrow \frac{L}{2\pi} \int_{-\infty}^{\infty} f(k_x) dk_x, \quad \text{as } L \rightarrow \infty. \end{aligned} \quad (127)$$

Exercise 26 Restore the \hbar in the prescription (126).

Using the prescription (126) we rewrite (123) in the thermodynamic limit as

$$\langle N \rangle = gV \int \frac{d^d \mathbf{k}}{(2\pi)^d} \frac{1}{e^{\beta(\epsilon_k - \mu)} - 1}. \quad (128)$$

We now use the fact that for free particles $\epsilon_k = k^2/2m$ and replace the integration over momenta by an integration over the energy variable. The way we introduce the so-called *density of states* (DOS) $\nu(\epsilon)$ via

$$\int \frac{d^d \mathbf{k}}{(2\pi)^d} f(|\mathbf{k}|) \equiv \int d\epsilon \nu(\epsilon) f(\epsilon). \quad (129)$$

Using the fact that for spherically symmetric functions the integration over the angular variables yields 4π , so that $d^3 \mathbf{k} = 4\pi k^2 dk$ we find (restoring the \hbar)

$$\nu(\epsilon) d\epsilon = \frac{m^{3/2}}{2^{1/2}\pi^2 \hbar^3} \epsilon^{1/2} d\epsilon \quad (d = 3). \quad (130)$$

Exercise 27 Find the DOS in $d = 2$ and $d = 1$. In $d = 2$ use the fact that for spherically symmetric functions $d^2 \mathbf{k} = 2\pi k dk$. Sketch the energy dependence of the DOS in $d = 1, 2, 3$, paying special attention to the $\epsilon \rightarrow 0$ region.

Combining (130) and (128) we find for the average density $n = \langle N \rangle/V$

$$n = g \frac{m^{3/2}}{2^{1/2}\pi^2 \hbar^3} \int_0^\infty \frac{\epsilon^{1/2} d\epsilon}{e^{\beta(\epsilon - \mu)} - 1}. \quad (131)$$

Similar manipulations can clearly be effected for other thermodynamic quantities as well. For example, consider the average energy. As compared to (123), Eq. (125) has an extra power of ϵ_k , therefore, applying (126) to (125), we find

$$\langle E \rangle = gV \frac{m^{3/2}}{2^{1/2}\pi^2\hbar^3} \int_0^\infty \frac{\epsilon^{3/2} d\epsilon}{e^{\beta(\epsilon-\mu)} - 1}. \quad (132)$$

Likewise, replacing the summation by integration in Eq. (122) we find for the grand potential

$$\Omega_{(\text{bosons})} = gV \frac{Tm^{3/2}}{2^{1/2}\pi^2\hbar^3} \int_0^\infty \epsilon^{1/2} \ln(1 - e^{-\beta(\epsilon-\mu)}) d\epsilon. \quad (133)$$

Integrating by parts the latter expression we find

$$\Omega_{(\text{bosons})} = -\frac{2}{3}gV \frac{m^{3/2}}{2^{1/2}\pi^2\hbar^3} \int_0^\infty \frac{\epsilon^{3/2} d\epsilon}{e^{\beta(\epsilon-\mu)} - 1}. \quad (134)$$

Comparing the latter expression with Eq. (132), we see that

$$\Omega_{\text{bosons}} = -(2/3) \langle E \rangle. \quad (135)$$

Exercise 28 *Derive analogs of Eqs. (131)–(135) for fermions. You will need a solution of Assignment 25. Comment on the similarities and differences between bosonic and fermionic cases.*

6.3 The Boltzmann limit

In this section we trace the relation between Bose and Fermi distributions with (presumably more familiar) Boltzmann distribution. To this end we consider (131), and introduce the dimensionless variable of integration $x = \epsilon/T$ so that

$$n = g \frac{(mT)^{3/2}}{2^{1/2}\pi^2\hbar^3} \int_0^\infty \frac{x^{1/2} dx}{e^{x-\beta\mu} \mp 1} \quad (136)$$

Here we anticipate the solution of Assignment 25 and generalize Eq. (131) so that it is applicable to both bosons [the upper sign in (136)] and fermions [the lower sign in (136)]. Notice that now the integral in the rhs of Eq. (136) is a dimensionless function of a dimensionless variable $\beta\mu$.

At this point we observe that the combination $n\hbar^3/(mT)^{3/2}$ is, up to a numerical factor, nothing but the third power of the ratio of the de Broglie wavelength, $\lambda \sim \hbar/(mT)^{1/2}$, to a mean interparticle distance, $\ell \sim n^{-1/3}$. Recall that it is in the limit $\lambda \ll \ell$ where the quantum mechanics gives way to the classical one. Therefore, on purely dimensional grounds we expect that in the classical limit the integral in the rhs of Eq. (136) will be small, which corresponds to $e^{-\beta\mu} \gg 1$, i.e.

$$\mu/T \rightarrow -\infty \quad (\text{Boltzmann limit.}) \quad (137)$$

Exercise 29 *Work out the explicit expression for $\mu(n, T)$ in the Boltzmann limit. Compare to the “semiclassical” results (eg Landau and Lifshitz, Statistical Mechanics I, Chap IV, Sec 45)*

Exercise 30 *Work out the virial corrections for the Bose or Fermi gases in the high temperature regime by expanding (136) in powers of the small factor $\exp(\beta\mu)$. Hence deduce the virial corrections to the energy and pressure. Interpret your results.*

6.4 Ideal Bose gas in the low-temperature regime: *Bose-Einstein condensation*

In this section we only consider spin-zero bosons, hence we put the spin degeneracy factor $g = 1$ in Eqs. (128)–(136).

We have already noted that Eq. (136) defines the chemical potential as an implicit function of the density and temperature. Working at fixed density, we start from the high-temperature limit, where μ is large and negative, cf (137). Lowering the temperature, μ grows monotonically (i.e. its absolute value diminishes). As we've seen in the previous section, the chemical potential must be negative. It turns out that μ reaches zero *at finite temperature*, T_0 , which can be found by setting $\mu = 0$ in Eq. (136):

$$n = \frac{(mT_0)^{3/2}}{2^{1/2}\pi^2\hbar^3} \int_0^\infty \frac{x^{1/2} dx}{e^x - 1} \quad (138)$$

The remaining integral is just a number, which can be expressed in terms of the known special functions using the formula

$$\int_0^\infty \frac{x^{p-1} dx}{e^x - 1} = \Gamma(p)\zeta(p) \quad (p > 1) ,$$

where $\Gamma(p)$ is the gamma-function and $\zeta(x)$ is the Riemann zeta-function. Using the numerical values for $\zeta(3/2)$ and $\Gamma(3/2)^3$, we find

$$T_0 \approx 3.31 \frac{\hbar^2}{m} n^{2/3} . \quad (139)$$

That is, Eq. (136) *does not have solutions with $\mu < 0$ for $T < T_0$* . This behavior is illustrated in Fig. 3. This situation leaves us in a quandary as we expect to be able to find a unique negative value of the chemical potential for any given T .

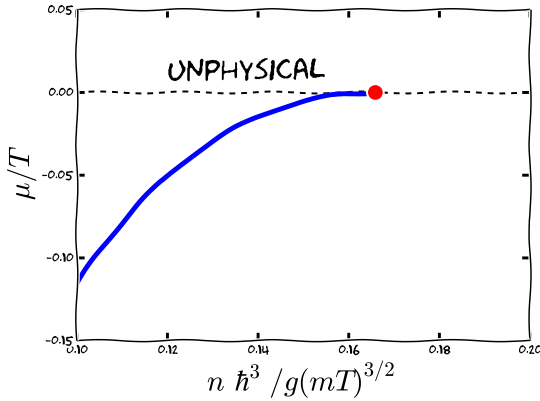


Figure 3: Chemical potential of the Bose gas as a function of the density and temperature.

The solution of this apparent contradiction is that our trick of replacing the sum, Eq. (123), by an integral, (128), breaks down at small μ . Indeed, as $e^{-\beta\mu}$ is large, the term in (123) with $\epsilon_k = 0$ is roughly of the same order of magnitude as other terms with small $\epsilon_k > 0$. On the other hand, as μ is small, the *single* level at $\epsilon_k = 0$ gives large contribution to the whole sum. Therefore, we expect a finite fraction of particles to occupy the single level at $\epsilon = 0$ —this phenomenon is known as *Bose-Einstein condensation*.

As we replace the sum by an integral, (128), and send $\mu \rightarrow 0$, the denominator of Eq. (128) goes to zero at $\epsilon \rightarrow 0$, so that we seem to have a divergence in the integral. In three dimensions though, the density of states, Eq. (130) goes to zero as $\epsilon \rightarrow 0$, hence the integral (128) converges, but *it misses the contribution of the ground state $\epsilon = 0$* .

Therefore, at $T < T_0$ we can separate the total number of particles into two contributions: those with $\epsilon = 0$ (the so-called Bose-Einstein condensate or simply *Bose condensate* or just *condensate*) and those with $\epsilon > 0$ (typically referred to as the “uncondensed particles”). At zero temperature

³For a reference, $\Gamma(3/2) = \sqrt{\pi}/2$, $\Gamma(5/2) = (3/2)\Gamma(3/2)$, $\zeta(3/2) \approx 2.61$, $\zeta(5/2) = 1.34$.

we expect all the particles to occupy the ground state, while at finite temperature we expect the two contributions to be of the same order of magnitude. The density of particles with $\epsilon > 0$ is given by (136) with $\mu = 0$, so that

$$n_{\epsilon>0} = \frac{(mT)^{3/2}}{2^{1/2}\pi^2\hbar^3} \int_0^\infty \frac{x^{1/2} dx}{e^x - 1} \quad \text{using (138)} \quad (140)$$

$$= n \left(\frac{T}{T_0} \right)^{3/2}. \quad (141)$$

The rest of the particles are in the condensate. The condensate density is given by the difference between the total density and the density of uncondensed particles, (141), that is,

$$n_{\epsilon=0} = n - n_{\epsilon>0} = n \left[1 - \left(\frac{T}{T_0} \right)^{3/2} \right]. \quad (142)$$

We thus see that the condensate density approaches the total density as $T \rightarrow 0$ and disappears as $T \rightarrow T_0$.

Exercise 31 *Investigate if Bose condensation is possible at finite temperature in one spatial dimension. Hint: using the DOS you've found in Assignment 27, derive the analog of Eq. (136). Then send the chemical potential to zero and investigate if the resulting integral converges.*

Exercise 32 *Repeat the Assignment 31 in two spatial dimensions.*

We now investigate the temperature dependence of the thermodynamic functions of the Bose gas in presence of the condensate. We focus on one of the measurable quantities— the heat capacity.

6.5 Heat capacity of the Bose gas in presence of the condensate

In this section we again focus on spin-zero bosons, thus the spin degeneracy factor $g = 1$. By definition, the heat capacity is defined as the temperature derivative of the energy:

$$c_V = \left(\frac{\partial \langle E \rangle}{\partial T} \right)_{N,V}, \quad (143)$$

where the derivative is done keeping the volume *and number of particles* fixed. The average energy is given by (125), where the thermal averages of the occupation numbers are given by (123).

We start by considering the temperature range $T < T_0$. In this regime, a fraction of the particles is in the condensate, i.e. these particles all occupy the zero-energy state, and add no contribution to the average energy of the gas. The rest of the energy levels are occupied according to the Bose distribution (123) with $\mu = 0$.

Therefore, we write

$$\begin{aligned} \langle E \rangle &= \sum_k \epsilon_k \bar{n}_k && \text{(replacing the sum by an integral, cf. Eq. (126))} \\ &= V \int \frac{d^d \mathbf{k}}{(2\pi)^d} \frac{\epsilon_k}{e^{\beta \epsilon_k} - 1} && \text{(introducing the DOS, Eq. (129))} \\ &= V \int_0^\infty \nu(\epsilon) d\epsilon \frac{\epsilon}{e^{\beta \epsilon} - 1} && (144) \end{aligned}$$

Using the explicit form of the DOS in three spatial dimensions, Eq. (130), and introducing the dimensionless variable $x = \beta\epsilon$, we find

$$\begin{aligned}\langle E \rangle &= \frac{m^{3/2}}{2^{1/2}\pi^2\hbar^3} \int_0^\infty d\epsilon \frac{\epsilon^{3/2}}{e^{\epsilon/T} - 1} \\ &= \frac{m^{3/2}VT^{5/2}}{2^{1/2}\pi^2\hbar^3} \int_0^\infty dx \frac{x^{3/2}}{e^x - 1} \\ &= \left(\frac{\Gamma(5/2)\zeta(5/2)}{2^{1/2}\pi^2} \right) \frac{m^{3/2}}{\hbar^3} VT^{5/2} .\end{aligned}\tag{145}$$

The precise value of the numerical coefficient in brackets is not terribly important (and can be easily calculated if necessary). What is important is the temperature dependence of the energy, $\langle E \rangle \propto T^{5/2}$, which immediately translates into the temperature dependence of the heat capacity:

$$c_V \propto T^{3/2} \quad (T < T_0) .\tag{146}$$

An interesting question now is what is the behavior of thermodynamic functions at the transition point $T = T_0$. To investigate this, we need to work out the thermodynamics at temperatures slightly above the transition. To this end, we need to take into account the temperature dependence of the chemical potential for $T \rightarrow T_0 + 0$. The latter is governed by Eq. (136), where we know that μ must be small and negative, so that we need to expand (136) as $\mu \rightarrow -0$. We cannot expand the right-hand side of (136) directly because we know that the main contribution to the integral comes from the region of the low energies. We thus employ a standard trick: to add and subtract something such that the main contribution to the integral is taken care of properly. To lighten the notation we define a shorthand notation

$$\xi = \frac{m^{3/2}}{2^{1/2}\pi^2\hbar^3} ,$$

and add and subtract from Eq. (136) its right-hand side with $\mu = 0$ (which we call N_0). Explicitly,

$$N_0 \equiv \xi VT^{3/2} \int_0^\infty \frac{x^{1/2} dx}{e^x - 1} ,\tag{147}$$

and we rewrite Eq. (136) identically as

$$N = N_0 + \xi VT^{3/2} \int_0^\infty \left(\frac{1}{e^{x-\beta\mu} - 1} - \frac{1}{e^x - 1} \right) x^{1/2} dx .\tag{148}$$

Keeping in mind that for $\beta\mu \rightarrow -0$ the relevant region of x is at the lower limit of integration, hence we expand the function under the integral in both x and $\beta\mu$:

$$x^{1/2} \left(\frac{1}{e^{x-\beta\mu} - 1} - \frac{1}{e^x - 1} \right) \approx x^{1/2} \left(\frac{1}{x - \beta\mu} - \frac{1}{x} \right) = \frac{\beta\mu}{x^{1/2}(x - \beta\mu)} ,$$

thus

$$N - N_0 = \xi VT^{1/2} \mu \int_0^\infty \frac{dx}{x^{1/2}(x - \beta\mu)} .\tag{149}$$

To do the integral in the last equation we use the substitution $y = \sqrt{x}$, and remember that $\mu < 0$ so that $\mu = -|\mu|$. We obtain

$$N - N_0 = -\pi\xi VT\sqrt{|\mu|} ,\tag{150}$$

therefore

$$\mu = - \left(\frac{N_0 - N}{\pi\xi VT} \right)^2 \quad (T \rightarrow T_0 + 0) ,\tag{151}$$

which explicitly defines the temperature dependence of μ in the limit specified. Notice that for $T \rightarrow T_0 + 0$ we have $\mu \rightarrow -0$, and $N - N_0 \rightarrow 0$.

We now expand the energy dependence on the chemical potential up to the first order:

$$E \approx E_0 + \frac{\partial E}{\partial \mu} \mu ,$$

where E_0 is the energy at $\mu = 0$, which is explicitly given by (145). Using (135) we have

$$\frac{\partial E}{\partial \mu} = -\frac{3}{2} \frac{\partial \Omega}{\partial \mu} = \frac{3}{2} N ,$$

so that

$$E = \begin{cases} E_0 - \frac{3}{2} N \left(\frac{N_0 - N}{\pi \xi V T} \right)^2 , & T \rightarrow T_0 + 0 , \\ E_0 , & T \rightarrow T_0 - 0 . \end{cases} \quad (152)$$

where we took into account the fact that just below the T_0 the total energy is nothing but E_0 .

There are several conclusions we can immediately draw from (152). First of all, we see that *the energy is a continuous function of temperature as $T \rightarrow 0$* . (Indeed, Eq.(151) shows that $N - N_0 \rightarrow 0$ as $T \rightarrow T_0 + 0$.) Moreover, the temperature derivative of energy—the heat capacity—is also continuous. It is only the derivative of the heat capacity which is discontinuous at $T = T_0$. The jump of the $\partial c_V / \partial T$ is nothing but the second derivative of the second term in (152), evaluated at $T = T_0$. To calculate this derivative at $T = T_0$ we only need to differentiate $N_0 - N$ (since other terms would contain $N - N_0$ and thus vanish at T_0), and we obtain

$$\Delta \left(\frac{\partial c_V}{\partial T} \right) = -3 \frac{N}{(\pi \xi V T)^2} \left(\frac{\partial N_0}{\partial T} \right)^2 \Big|_{T=T_0} . \quad (153)$$

Using the definition of N_0 , Eq. (147) we can perform the derivative explicitly, and we finally obtain

$$\Delta \left(\frac{\partial c_V}{\partial T} \right) = -\frac{27}{4\pi^2} \left(\zeta(3/2) \Gamma(3/2) \right)^2 \frac{N}{T_0} . \quad (154)$$

Evaluating the numerical factors we find the following behavior of the heat capacity: for $T < T_0$ is grows monotonically according to Eq. (146), and at $T = T_0$ it has a cusp, where the sign of the derivative changes.

Exercise 33 Consider a three-dimensional gas of spinless bosons with linear dispersion $\epsilon_{\mathbf{k}} = c|\mathbf{k}|$, where \mathbf{k} is momentum and c has the units of velocity, so that the Hamiltonian takes the form $\hat{H} = \sum_{\mathbf{k}} c|\mathbf{k}| \hat{n}_{\mathbf{k}}$. Assuming $\mu = 0$, calculate the temperature dependence of the heat capacity. Hint: start from Eq. (125).