

Chapter 6

Bosons and fermions at finite temperature

After reviewing some statistical mechanics in Sec. 6.1, the occupation number representation is employed to derive some standard results for noninteracting bosons and fermions at finite temperature. The phenomenon of Bose-Einstein condensation is discussed in Sec. 6.2. Bosons in an infinite homogeneous system are considered in Sec. 6.2.1 while a preliminary discussion Bose-Einstein condensation in traps is given in Sec. 6.2.2 and in the thermodynamic limit in Sec. 6.2.3. Fermions at finite temperature are briefly considered in Sec. 6.3.

6.1 Some statistical mechanics

A microscopic description of a system at finite temperature can be obtained by evaluating the ensemble average of the statistical operator. We will consider the statistical operator in the grand canonical ensemble

$$\hat{\rho}_G = \frac{e^{-\beta(\hat{H} - \mu\hat{N})}}{Z_G}, \quad (6.1)$$

where $\beta = (k_B T)^{-1}$, μ is the chemical potential, and the grand partition function is given by

$$\begin{aligned} Z &= \text{Tr} \left(e^{-\beta(\hat{H} - \mu\hat{N})} \right) = \\ &= \sum_N \sum_n \langle \Psi_n^N | e^{-\beta(\hat{H} - \mu\hat{N})} | \Psi_n^N \rangle = \sum_N \sum_n e^{-\beta(E_n^N - \mu N)}, \end{aligned} \quad (6.2)$$

where in the evaluation of the trace the basis with energy and particle number eigenstates was considered. A standard result from statistical mechan-

ics [Landau and Lifshitz (1980)] then yields the thermodynamic potential

$$\Omega(T, V, \mu) = -k_B T \ln Z, \quad (6.3)$$

so that one can rewrite the statistical operator as

$$\hat{\rho}_G = e^{\beta(\Omega - \hat{H} + \mu \hat{N})}. \quad (6.4)$$

The ensemble average $\langle \hat{O} \rangle$ of any operator \hat{O} is then obtained by evaluating

$$\langle \hat{O} \rangle = \text{Tr} \left(\hat{\rho}_G \hat{O} \right) = \text{Tr} \left(e^{\beta(\Omega - \hat{H} + \mu \hat{N})} \hat{O} \right) = \frac{\text{Tr} \left(e^{-\beta(\hat{H} - \mu \hat{N})} \hat{O} \right)}{\text{Tr} \left(e^{-\beta(\hat{H} - \mu \hat{N})} \right)}. \quad (6.5)$$

Detailed results can be obtained by considering noninteracting many-fermion or many-boson systems. By replacing \hat{H} by \hat{H}_0 one can use the complete set of states of the independent particle model in the occupation number representation to evaluate the corresponding grand partition function. It is helpful to use the notation of Eqs. (2.18) and (2.19) introduced for fermions and bosons, respectively. Summing over the complete set of states in Fock space can then be accomplished by summing over all possible occupations of the sp states with no restrictions for bosons but limiting the occupation to zero or one for fermions. The operator \hat{H}_0 describing the energy and the number operator can then be replaced by their eigenvalues for a given state as follows

$$\hat{H}_0 |n_1 \dots n_\infty\rangle = \sum_i n_i \varepsilon_i |n_1 \dots n_\infty\rangle \quad (6.6)$$

$$\hat{N} |n_1 \dots n_\infty\rangle = \sum_i n_i |n_1 \dots n_\infty\rangle. \quad (6.7)$$

As a result one obtains for the grand partition function

$$\begin{aligned} Z_0 &= \sum_{n_1 \dots n_\infty} \exp \{ \beta(\mu n_1 - \varepsilon_1 n_1) \} \dots \exp \{ \beta(\mu n_\infty - \varepsilon_\infty n_\infty) \} \\ &= \prod_{i=1}^{\infty} \text{Tr} \exp \{ -\beta(\varepsilon_i - \mu) n_i \}, \end{aligned} \quad (6.8)$$

where the trace corresponds to summing over all occupation numbers for sp state i . For bosons one must consider all occupation numbers and one therefore obtains

$$Z_0^B = \prod_{i=1}^{\infty} \sum_{n=0}^{\infty} [\exp \{ \beta(\mu - \varepsilon_i) \}]^n = \prod_{i=1}^{\infty} [1 - \exp \{ \beta(\mu - \varepsilon_i) \}]^{-1}. \quad (6.9)$$

The corresponding thermodynamic potential for noninteracting bosons is therefore given by

$$\begin{aligned}\Omega_0^B(T, V, \mu) &= -k_B T \ln \prod_{i=1}^{\infty} [1 - \exp \{\beta(\mu - \varepsilon_i)\}]^{-1} \\ &= k_B T \sum_{i=1}^{\infty} \ln [1 - \exp \{\beta(\mu - \varepsilon_i)\}].\end{aligned}\quad (6.10)$$

The average number of particles can now be obtained by differentiating the thermodynamic potential with respect to the chemical potential keeping T and V (meaning ε_i) fixed [Landau and Lifshitz (1980)] and including an extra minus sign

$$\langle N \rangle \equiv \sum_{i=1}^{\infty} n_i^0 = \sum_{i=1}^{\infty} \frac{1}{\exp \{\beta(\varepsilon_i - \mu)\} - 1},\quad (6.11)$$

where the mean occupation number of a sp state i is denoted by n_i^0 .

For fermions the occupation number is restricted to 0 or 1, and the corresponding grand partition function is obtained by taking only those terms in Eq. (6.8)

$$Z_0^F = \prod_{i=1}^{\infty} \sum_{n=0}^1 [\exp \{\beta(\mu - \varepsilon_i)\}]^n = \prod_{i=1}^{\infty} [1 + \exp \{\beta(\mu - \varepsilon_i)\}].\quad (6.12)$$

The thermodynamic potential for noninteracting fermions is therefore given by

$$\Omega_0^F(T, V, \mu) = -k_B T \sum_{i=1}^{\infty} \ln [1 + \exp \{\beta(\mu - \varepsilon_i)\}],\quad (6.13)$$

with the number of particles now given by

$$\langle N \rangle \equiv \sum_{i=1}^{\infty} n_i^0 = \sum_{i=1}^{\infty} \frac{1}{\exp \{\beta(\varepsilon_i - \mu)\} + 1},\quad (6.14)$$

We note that the average occupation numbers of a sp state i , given by n_i^0 , has the familiar form for bosons in Eq. (6.11) and for fermions in Eq. (6.14).

6.2 Bosons at finite T

6.2.1 Bose-Einstein condensation in infinite systems

The ground state of a noninteracting system of bosons is obviously the one in which all the bosons occupy the lowest sp level. This state is the limit that one approaches when the temperature is lowered towards $T = 0$. First we will consider a collection of bosons in a box (with the usual periodic boundary conditions). The sp energy is therefore given by

$$\varepsilon(k) = \frac{\hbar^2 k^2}{2m}. \quad (6.15)$$

Summing over sp states can then be replaced by an integral over wavenumbers as discussed in Ch.5

$$\sum_i \rightarrow \frac{\nu V}{(2\pi)^3} \int d^3 k, \quad (6.16)$$

where ν is the degeneracy factor associated with discrete quantum numbers like spin. It is common to transform the integral over k to one over the energy given by Eq. (6.15)

$$\frac{\nu V}{(2\pi)^3} 4\pi k^2 dk = \frac{\nu V}{2\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} \frac{\varepsilon d\varepsilon}{2\varepsilon^{1/2}} = \frac{\nu V}{4\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} \varepsilon^{1/2} d\varepsilon. \quad (6.17)$$

One can now write the thermodynamic potential for an ideal Bose gas as

$$\begin{aligned} \Omega_0^B &= k_B T \frac{\nu V}{4\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} \int_0^\infty d\varepsilon \varepsilon^{1/2} \ln [1 - \exp \{\beta(\mu - \varepsilon)\}] \\ &= -\frac{\nu V}{4\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} \frac{2}{3} \int_0^\infty d\varepsilon \frac{\varepsilon^{3/2}}{\exp \{\beta(\varepsilon - \mu)\} - 1}, \end{aligned} \quad (6.18)$$

where in the last line a partial integration has been performed. Similarly one obtains for the average energy

$$E = \sum_i n_i^0 \varepsilon_i = \frac{\nu V}{4\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} \int_0^\infty d\varepsilon \frac{\varepsilon^{3/2}}{\exp \{\beta(\varepsilon - \mu)\} - 1}, \quad (6.19)$$

and average particle number

$$N = \sum_i n_i^0 = \frac{\nu V}{4\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} \int_0^\infty d\varepsilon \frac{\varepsilon^{1/2}}{\exp \{\beta(\varepsilon - \mu)\} - 1}. \quad (6.20)$$

Using $\Omega = -PV$ one recovers from Eqs. (6.18) and (6.19) the standard result for an ideal gas $PV = \frac{2}{3}E$. The denominator in the integrals above reflects the occupation probability associated with energy ε . As such this denominator may not become negative. For this reason μ must always be such that for a given sp Hamiltonian with a corresponding spectrum $\varepsilon - \mu \geq 0$ (for any ε). In the present case ε may be zero so $\mu \leq 0$. If the density in Eq. (6.20) is kept fixed while the temperature is lowered one expects the absolute value of the chemical potential to decrease to allow the density to remain fixed. The limit $\mu = 0$ is then reached for a temperature T_0 for which Eq. (6.20) yields

$$\begin{aligned} N &= \frac{\nu V}{4\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} \int_0^\infty d\varepsilon \frac{\varepsilon^{1/2}}{\exp\{\varepsilon/k_B T_0\} - 1} \\ &= \frac{\nu V}{4\pi^2} \left(\frac{2mk_B T_0}{\hbar^2} \right)^{3/2} \int_0^\infty dx \frac{x^{1/2}}{\exp(x) - 1} \\ &= \frac{\nu V}{4\pi^2} \left(\frac{2mk_B T_0}{\hbar^2} \right)^{3/2} \zeta\left(\frac{3}{2}\right) \frac{1}{2} \sqrt{\pi}, \end{aligned} \quad (6.21)$$

where $\zeta\left(\frac{3}{2}\right) = 2.612$ (Riemann ζ -function). The result can be rewritten as

$$T_0 = \frac{3.31}{\nu^{2/3}} \frac{\hbar^2}{mk_B} \left(\frac{N}{V} \right)^{2/3}. \quad (6.22)$$

For temperatures below T_0 it is clear that the integral will give only the number of particles with $\varepsilon > 0$ while the occupation of the lowest state can be expected to become macroscopically large. The latter state does not contribute to the integral due to $\sqrt{\varepsilon}$ weighting which occurs when one transforms from summation to integration. One must now explicitly keep track of the particles in the lowest sp state. Equation (6.21) with T_0 replaced by T continues to correspond to the number of particles with $\varepsilon > 0$ since μ remains zero. This means that one can write for $T < T_0$

$$N_{\varepsilon>0}(T) = N \left(\frac{T}{T_0} \right)^{3/2}. \quad (6.23)$$

The remaining particles must therefore be in the sp state with $\varepsilon = 0$ according to

$$N_{\varepsilon=0}(T) = N \left[1 - \left(\frac{T}{T_0} \right)^{3/2} \right]. \quad (6.24)$$

This macroscopic occupation of the lowest sp state is referred to as Bose-Einstein condensation. One can consult [Landau and Lifshitz (1980); Fetter and Walecka (1971)] that at T_0 there is discontinuity in the slope of the specific heat at constant volume. Using the density of ^4He atoms $\rho_4 = 0.145 \text{ g cm}^{-3}$ one finds $T_0 = 3.14 \text{ K}$ for the transition temperature. The actual experimental behavior is somewhat reminiscent of this result but the specific heat has the shape of a λ and is different from the ideal gas prediction. The experimental transition takes place at 2.2 K and below this temperature ^4He exhibits superfluid properties. It is not obvious that properties associated with superfluidity have anything to do with the above ideal gas description.

6.2.2 *Bose-Einstein condensation in traps*

The original papers by Bose and Einstein are discussed in context in [Pais (1986)]. Reviews from just before 1995 are collected in [Griffin *et al.* (1995)] while the more recent developments are discussed in [Dalfovo *et al.* (1999); Ketterle (1999); Burnett *et al.* (1999)]. New books on the subject have also been written recently [Pethick and Smith (2002); Pitaevskii and Stringari (2003)]. In 1995 Bose-Einstein condensation was first observed in experiments on rubidium (^{87}Rb) [Anderson *et al.* (1995)] and sodium (^{23}Na) atoms [Davis *et al.* (1995)] leading to the 2001 Nobel prize in physics awarded to Wieman, Cornell, and Ketterle. Both types of atoms have an odd number of protons and an even number of neutrons in the nucleus. Together with the odd number of electrons the total number of fermion constituents corresponds to an even integer which makes these atoms into boson particles (always for energies small compared to their internal excitation energies). Historically, the superfluidity of liquid ^4He has been linked to Bose-Einstein condensation. Evidence has been gathered experimentally from neutron scattering measurements at high momentum transfer (backed up by theoretical calculations) that the occupation of the lowest sp state in the liquid towards 0 K is close to 10% [Sokol (1995)]. This represents a macroscopic occupation of the lowest sp state (the zero momentum state). In the case of ^4He it is, however, hard to find an unambiguous signature of Bose-Einstein condensation. Only recently [Wyatt (1998)], has tentative evidence for the condensate in ^4He become available by using quantum evaporation. This technique involves the scattering of phonons (excitations generated in the liquid) with atoms somewhat analogous to the photoelectric effect. When such a phonon is incident on the free surface of the liquid,

it is absorbed by an atom which is released into the vacuum above the liquid with conservation of momentum parallel to the surface. Measuring the momentum of the phonon and the evaporated atom allows determination of the momentum of the atom in the liquid before it absorbed the phonon. The measurements of [Wyatt (1998)] at 100 mK indicate a macroscopic occupation of the zero momentum state but further refinements are necessary to pin down the actual fraction of condensed atoms.

The first efforts to achieve Bose-Einstein condensation with atomic gases were focused on experiments with hydrogen atoms. Only recently [Fried *et al.* (1998)] has Bose-Einstein condensation been observed for spin-polarized hydrogen. Critical to these new developments for atomic gases have been laser-based methods, such as laser cooling and magneto-optical trapping [Chu (1998); Cohen-Tannoudji (1998); Phillips (1998)]. After trapping, further lowering of the temperature can be obtained by evaporative cooling in which the depth of the trap is reduced allowing the most energetic atoms to escape while the remaining atoms rethermalize at lower temperature. It should be noted that these systems must be studied in a metastable gas phase since the equilibrium configuration is the solid phase (except for hydrogen). Typical temperatures achieved to study Bose-Einstein condensation ranges from 500 nK to 2 μ K with densities between 10^{14} and 10^{15} atoms cm^{-3} . The largest condensates in sodium have 20 million atoms and in hydrogen, 1 billion atoms. Condensates have also been obtained for ^7Li atoms [Bradley *et al.* (1995)]. Other vapors of caesium, potassium, and helium are under study. The shape of the condensates depends on the magnetic trap and can be round with a diameter of 10 to 50 μm , or cigar-shaped with a diameter of about 15 μm and a length of 300 μm .

The confinement in traps means that these systems are highly inhomogeneous (substantial density variation in a finite region of space). This implies that Bose-Einstein condensation can also be observed in coordinate space since the relevant sp wave functions are confined. The magnetic traps used for alkali atoms yield confining potentials that can be very well approximated by a quadratic form given by

$$V_{ext}(\mathbf{r}) = \frac{1}{2} m (\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2). \quad (6.25)$$

While for the actual analysis of the experimental data it is crucial to consider the interaction between the atoms as discussed in Ch. 12, one can obtain already very useful results by considering the atoms to be identical pointlike noninteracting particles in a harmonic potential given by

Eq. (6.25). The eigenvalues of the corresponding three-dimensional sp harmonic oscillator potential are given by

$$\varepsilon_{n_x n_y n_z} = (n_x + \frac{1}{2}) \hbar \omega_x + (n_y + \frac{1}{2}) \hbar \omega_y + (n_z + \frac{1}{2}) \hbar \omega_z, \quad (6.26)$$

where $\{n_x, n_y, n_z\}$ are non-negative integers. The ground state of the non-interacting system with N atoms is obtained by putting all atoms in the lowest sp state with $n_x = n_y = n_z = 0$. The corresponding sp wave function is simply the product of three ground state oscillator wave functions, one for each of the three dimensions considered. This wave function is given by

$$\phi_{000}(\mathbf{r}) = \left(\frac{m\omega_{HO}}{\pi\hbar} \right)^{3/4} \exp \left\{ -\frac{m}{2\hbar} (\omega_x x^2 + \omega_y y^2 + \omega_z z^2) \right\}, \quad (6.27)$$

where the geometric average of the oscillator frequencies has been used

$$\omega_{HO} = (\omega_x \omega_y \omega_z)^{1/3}. \quad (6.28)$$

The density distribution for the ground state with N such bosons

$$|\Phi_0^N\rangle = \frac{1}{\sqrt{N!}} (a_{000}^\dagger)^N |0\rangle, \quad (6.29)$$

then becomes

$$\rho(\mathbf{r}) = N |\phi_{000}(\mathbf{r})|^2, \quad (6.30)$$

which grows with N but the size of the cloud is independent of N and determined by the trap potential and the corresponding harmonic oscillator length:

$$a_{HO} = \left(\frac{\hbar}{m\omega_{HO}} \right)^{1/2}, \quad (6.31)$$

which corresponds to the average width of the Gaussian represented by Eq. (6.27). In the available experiments this important length scale is typically of the order $a_{HO} \approx 1 \mu\text{m}$. At finite temperature the atoms will also occupy excited states of the oscillator potential. The radius of this cloud will be larger than a_{HO} . This effect can be estimated by using the classical Boltzmann distribution for the density for a spherical potential $V_{ext}(r)$ [Landau and Lifshitz (1980)]

$$\rho_{cl}(r) \propto \exp \left\{ -\frac{V_{ext}(r)}{k_B T} \right\}. \quad (6.32)$$

If

$$V_{ext}(r) = \frac{1}{2}m\omega_{HO}^2 r^2, \quad (6.33)$$

the width of the classical density distribution is given by

$$R_T = a_{HO} \left(\frac{k_B T}{\hbar\omega_{HO}} \right)^{1/2}, \quad (6.34)$$

and therefore larger than a_{HO} . This consideration illustrates that Bose-Einstein condensation in harmonic traps shows up in the form of a sharp peak in the central region of the density distribution. By taking the Fourier transform of the ground state wave function, one obtains the momentum distribution of the atoms in the condensate. Since the wave function in momentum space is also Gaussian, this distribution is centered at zero momentum with a width proportional to a_{HO}^{-1} . This means that the condensate appears both in coordinate and momentum space as a narrow peak. Note that this is quite different from the case of a uniform gas where the particles go to the zero momentum state, but there is no signature in coordinate space since condensed and noncondensed particles fill the same volume. The experimental signal of Bose-Einstein condensation has been detected as the occurrence of a sharp peak over a broader distribution in both the velocity and spatial distributions. By switching off the trap, one lets the condensate expand and measures the density of the expanding cloud by light absorption. If there is no interaction between the atoms, the expansion is ballistic and one can relate the imaged distribution to the initial velocity (momentum) distribution. For the spatial distribution one measures the density of the atoms in the trap directly by dispersive light scattering. It should be kept in mind that the effect of the interaction between the atoms modifies the results substantially. Nevertheless important signatures identifiable at the noninteracting level persist related to the symmetry of the confining potential when interactions are taken into account. The first experiments were carried out with axial symmetry for which one can write the ground state wave function as

$$\phi_{000}(\mathbf{r}) = \frac{\lambda^{1/4}}{\pi^{3/4} a_{\perp}^{3/2}} \exp \left\{ -\frac{1}{2a_{\perp}^2} (r_{\perp}^2 + \lambda z^2) \right\}, \quad (6.35)$$

where $a_{\perp} = (\hbar/m\omega_{\perp})^{1/2}$ is the oscillator length in the xy -plane and, since $\omega_{\perp} = \lambda^{-1/3}\omega_{HO}$, one also has $a_{\perp} = \lambda^{1/6}a_{HO}$. The momentum space wave function has a corresponding asymmetry governed by the parameter

λ . If condensation has taken place, the shape of the expanding cloud is an ellipse with an aspect ratio of $\sqrt{\lambda}$ whereas one expects spherical symmetry in the case of a thermal distribution. The actual values of this ratio is strongly influenced by the interaction between the atoms but still shows this important anisotropy which is used to identify the condensate.

6.2.3 Trapped bosons at finite temperature: thermodynamic limit

At temperature T the number of particles is given by Eq. (6.11) which yields in the present case

$$N = \sum_{n_x n_y n_z} \frac{1}{\exp\{\beta(\varepsilon_{n_x n_y n_z} - \mu)\} - 1}, \quad (6.36)$$

while the total energy is given by

$$E = \sum_{n_x n_y n_z} \frac{\varepsilon_{n_x n_y n_z}}{\exp\{\beta(\varepsilon_{n_x n_y n_z} - \mu)\} - 1}. \quad (6.37)$$

Statistical mechanics is complicated by the fact that the usual thermodynamic limit is not appropriate for these gases. Indeed due to the inhomogeneity of the system it is not possible to take N and V to infinity while keeping the ratio constant. As in the uniform case, however, one may separate the lowest energy ε_{000} from the sum in Eq. (6.36) and denote by N_0 the number of particles in this state. This number can be of order N when the chemical potential becomes equal to the energy of the lowest state

$$\mu \rightarrow \mu_c = \frac{3}{2}\hbar\bar{\omega}, \quad (6.38)$$

where $\bar{\omega} = (\omega_x + \omega_y + \omega_z)/3$ is the average frequency. Using this result one may write

$$N - N_0 = \sum_{n_x n_y n_z \neq 0} \frac{1}{\exp\{\beta\hbar(\omega_x n_x + \omega_y n_y + \omega_z n_z)\} - 1}. \quad (6.39)$$

One may evaluate this sum numerically for finite N but for $N \rightarrow \infty$ the sum can be replaced by an integral

$$N - N_0 = \int_0^\infty dn_x dn_y dn_z \frac{1}{\exp\{\beta\hbar(\omega_x n_x + \omega_y n_y + \omega_z n_z)\} - 1}. \quad (6.40)$$

This approximation is referred to as a semiclassical description of the excited states since it implies that the relevant excitation energies are much

larger than the level spacing which is fixed by the oscillator frequencies. It is expected to be good for large N and $k_B T \gg \hbar\omega_0$ but can always be checked numerically using Eq. (6.39). The integral (6.40) can be evaluated with the following result

$$N - N_0 = \zeta(3) \left(\frac{k_B T}{\hbar\omega_{HO}} \right)^3, \quad (6.41)$$

where the Riemann ζ function is given by $\zeta(3) \approx 1.202$ and ω_{HO} is the geometric average defined earlier. From this result one can obtain the transition temperature for Bose-Einstein condensation. By imposing that $N_0 \rightarrow 0$ at T_c^0 one obtains

$$k_B T_c^0 = \hbar\omega_{HO} \left(\frac{N}{\zeta(3)} \right)^{1/3} = 0.94 \hbar\omega_{HO} N^{1/3}. \quad (6.42)$$

One can use this result in Eq. (6.41) to obtain the T dependence of the condensate fraction for $T < T_c^0$

$$\frac{N_0}{N} = 1 - \left(\frac{T}{T_c^0} \right)^3. \quad (6.43)$$

By evaluating the energy in a similar way one may obtain all thermodynamic quantities. A further useful result is the density of thermal particles (out of the condensate) $\rho_T(\mathbf{r})$. The sum of $\rho_T(\mathbf{r})$ and the condensate density, $\rho_0(\mathbf{r}) = N_0 |\phi_{000}(\mathbf{r})|^2$ gives the total density distribution. One may use the classical expression in this case

$$\rho_T(\mathbf{r}) = \int \frac{d\mathbf{p}}{(2\pi\hbar)^3} [\exp\{\beta\epsilon(\mathbf{p}, \mathbf{r})\} - 1]^{-1}, \quad (6.44)$$

where

$$\epsilon(\mathbf{p}, \mathbf{r}) = \frac{\mathbf{p}^2}{2m} + V_{ext}(\mathbf{r}) \quad (6.45)$$

is the semiclassical energy in phase space. Equation 6.44 then yields

$$\rho_T(\mathbf{r}) = \frac{g_{3/2}(e^{-\beta V_{ext}(\mathbf{r})})}{\lambda_T^3}, \quad (6.46)$$

where the function $g_{3/2}$ is discussed in [Huang (1987)]. While there are important finite size corrections and crucial modifications of these results when the interaction between the atoms is taken into account [Dalfovo *et al.* (1999)], the above results involving noninteracting bosons already give

the main ideas relevant for the understanding of the recent experiments on Bose-Einstein condensation.

6.3 Fermions at finite T

6.3.1 Noninteracting fermion systems

The noninteracting Fermi gas at finite temperature yields thermodynamic quantities that exhibit characteristic differences with their bosonic counterparts. Using fermion occupation numbers one obtains for the thermodynamic potential of the homogeneous Fermi gas after performing similar steps as in the noninteracting Bose gas

$$\Omega_0^F = -\frac{\nu V}{4\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} \frac{2}{3} \int_0^\infty d\varepsilon \frac{\varepsilon^{3/2}}{\exp\{\beta(\mu - \varepsilon)\} + 1}. \quad (6.47)$$

Similarly, one obtains for the energy

$$E = \sum_i n_i^0 \varepsilon_i = \frac{\nu V}{4\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} \int_0^\infty d\varepsilon \frac{\varepsilon^{3/2}}{\exp\{\beta(\varepsilon - \mu)\} + 1}, \quad (6.48)$$

and particle number

$$N = \sum_i n_i^0 = \frac{\nu V}{4\pi^2} \left(\frac{2m}{\hbar^2}\right)^{1/2} \int_0^\infty d\varepsilon \frac{\varepsilon^{1/2}}{\exp\{\beta(\varepsilon - \mu)\} + 1}. \quad (6.49)$$

Using $\Omega = -PV$ one recovers from Eqs. (6.47) and (6.48) also for fermions the standard result for an ideal gas $PV = \frac{2}{3}E$. The denominator in the integrals above reflects the occupation probability associated with energy ε . It is clear that this occupation number is always less or equal to one for all values of μ and T . It is useful to check the zero-temperature limit which recovers the result obtained in the previous section with $\mu = \varepsilon_F$ at $T = 0$. Relevant thermodynamic quantities are straightforward to obtain [Fetter and Walecka (1971); Landau and Lifshitz (1980)].

6.3.2 Fermion atoms in traps

While the transition to a Bose-Einstein condensate for atomic gases is abrupt, the crossover to quantum degeneracy for fermionic atoms is gradual. It has recently been demonstrated for the first time for ^{40}K atoms

[DeMarco and Jin (1999)]. This potassium atom has an odd number of protons, neutrons, and electrons thereby making it a fermion. The electrons combine to atomic spin $F = 9/2$. It is more difficult to cool fermions by using the evaporation technique mentioned earlier. In this process the highest energy atoms are removed and the remaining gas equilibrates by elastic collisions at a lower temperature. This elastic collision rate drops sharply for fermions when the temperature is lowered because of the interaction is dominated by the S -wave. This S -wave scattering is prohibited for single species fermions as discussed in Ch. 5. This problem was overcome by using a mixture of two spin states for which S -wave collisions are allowed. For the trap used in the experiment one expects a Fermi temperature of $0.6 \mu\text{K}$. The actual experiment cooled about 8×10^5 atoms to about $T = 0.5T_F$. At that point one of the spin states was removed and a single-component gas remained.

One may proceed in a similar fashion as for bosons to describe the sp hamiltonian for the fermions

$$H = \frac{p_x^2 + p_y^2 + p_z^2}{2m} + \frac{1}{2}m\omega_r^2(x^2 + y^2 + \lambda^2 z^2), \quad (6.50)$$

where ω_r and $\omega_z = \lambda\omega_r$ are the trap frequencies in the radial and axial directions, respectively. The sp energy is given by Eq. (6.26) with appropriate changes in notation for the oscillator frequencies. In the actual experiments the thermal energies far exceed the level spacing ($k_B T \gg \hbar\omega_r$) as for the boson systems discussed above. One may therefore replace the discrete sp spectrum with a continuous one employing the appropriate density of states. The density of states at ϵ can be expressed in general as [Economou (1983)]

$$\rho(\epsilon) = \sum_n \delta(\epsilon - \epsilon_n), \quad (6.51)$$

where ϵ_n is given by the spectrum under consideration. One can show that for the spectrum corresponding to the hamiltonian given by Eq. (6.50) one obtains

$$\rho(\epsilon) = \frac{\epsilon^2}{2\lambda(\hbar\omega_r)^3}. \quad (6.52)$$

A practical way to obtain this density is to first calculate the number of states with energy below $\epsilon + d\epsilon$, then subtract the number below ϵ , and then divide by $d\epsilon$ (for $d\epsilon \rightarrow 0$). One can now use the fermion equivalent of

Eq. (6.36) to study the chemical potential [Butts and Rokhsar (1997)]

$$\begin{aligned} N &= \sum_{n_x n_y n_z} [\exp \{ \beta(\varepsilon_{n_x n_y n_z} - \mu) \} + 1]^{-1} \\ &= \int d\varepsilon \frac{\rho(\varepsilon)}{e^{\beta(\mu - \varepsilon)} + 1}. \end{aligned} \quad (6.53)$$

At zero temperature all levels below the Fermi energy are occupied, the ones above empty. Integrating Eq. (6.53) then gives

$$\varepsilon_F \equiv \mu(T = 0, N) = \hbar\omega_r [6\lambda N]^{1/3} \quad (6.54)$$

which yields the energy scale for the atomic cloud. A characteristic length scale is given by the extend of the orbit of a classical particle with energy ε_F in the trap potential

$$R_F \equiv \left[\frac{2\varepsilon_F}{m\omega_r^2} \right]^{1/2} = (48\lambda N)^{1/6} a_r, \quad (6.55)$$

where a_r is the radial oscillator parameter. A characteristic wave number is obtained from the momentum of a particle with energy ε_F

$$k_F \equiv \left[\frac{2m\varepsilon_F}{\hbar^2} \right]^{1/2} = (48\lambda N)^{1/6} \frac{1}{a_r} = \frac{48\lambda N^{1/3}}{R_F^3}, \quad (6.56)$$

which shows that the k_F is of the size of the interparticle spacing in the gas. For general temperature, one can determine the chemical potential numerically from Eq. (6.53). Analytic results can be obtained at low temperature ($k_B T \ll \varepsilon_F$) from Sommerfeld's expansion [Landau and Lifshitz (1980)]

$$\mu(T, N) = \varepsilon_F \left[1 - \frac{\pi^2}{3} \left(\frac{k_B T}{\varepsilon_F} \right)^2 \right]. \quad (6.57)$$

In the classical limit ($k_B T \gg \varepsilon_F$), one finds

$$\mu(T, N) = -k_B T \ln \left[6 \left(\frac{k_B T}{\varepsilon_F} \right)^3 \right]. \quad (6.58)$$

Obtaining the energy in a similar fashion, one may then obtain the specific heat of the trapped gas from

$$C_N \equiv \frac{1}{N} \left. \frac{\partial E}{\partial T} \right|_N, \quad (6.59)$$

where $E(T, N)$ is the total energy of the gas. The experimental data from [DeMarco and Jin (1999)] clearly confirm the expectations for the deviations of the energy from the classical result as a function of temperature as well as the behavior of the specific heat given by Eq. (6.59). Further experiments are geared towards studying situations in which the interaction between atoms near the Fermi energy is effectively attractive. One expects to be able to learn a lot about pairing properties from such systems.

6.4 Exercises

- (1) Calculate the energy and corresponding specific heat at constant volume of the noninteracting Bose gas below and above T_0 .
- (2) Calculate the energy of a trapped Bose gas, the corresponding specific heat and compare these quantities with those from the uniform Bose gas.
- (3) Provide the details for the calculation of the density of states given in Eq. (6.52). Use Sommerfeld's expansion to determine the energy of the Fermi gas in the trap at low temperature and calculate the specific heat according to Eq. (6.59). Compare your results with [DeMarco and Jin (1999)].

