

Atomic hydrogen in magnetostatic traps

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LECTURE NOTES

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Introduction

This course deals with the properties of atomic quantum gases at ultra-low temperatures and atomic hydrogen as a primary example. As hydrogen is known, to the public at large, mostly for the various ways in which it participates in violent processes, it must be emphasised right from the start that we will meet in this course atomic hydrogen as a delicate substance that behaves much alike an inert gas. In the four oral lectures presented in Stirling, three topics were emphasised: (a) the position of hydrogen among the quantum gases, (b) experiments with magnetically trapped hydrogen and (c) quantum adsorption of atomic hydrogen on the surface of liquid helium. In the written version of these lectures the attention is concentrated on the first two topics. The third topic has been described in educational detail by the present author in the lecture notes of the Les Houches summer school of 1990 [1].

Rather than outlining the peculiarities of atomic hydrogen, emphasis will be put on general properties of quantum gases. Building on the extensive experience of various research groups with the low temperature gas phase of atomic hydrogen, many interesting aspects could be illustrated with well established (and sometimes very familiar) experimental and theoretical results. The main topics of the course are described in two sections: properties of weakly interacting Bose gases in external potential fields (section 2) and evaporative cooling (section 3) as a prominent method to achieve ultra-low temperatures in trapped atomic gases. The text starts with an introductory summary of basic properties of spin-polarised hydrogen. Comprehensive reviews that may serve for further introduction to atomic hydrogen *as a quantum gas* were written by Greytak and Kleppner [2] and by Silvera and Walraven [3]. Also several articles in the book *Bose-Einstein Condensation* [4] may be valuable to meet the dilute Bose gases in a broader context.

In the final stages of preparation of the manuscript the observation of Bose-Einstein condensation in ultra-cold atomic rubidium vapor was announced by Cornell and Wieman at JILA in Boulder [5]. This exciting result adds a very timely aspect to the article. It is hoped that the emphasis on general properties will make the paper valuable to a wide audience as an introduction to a fascinating field.

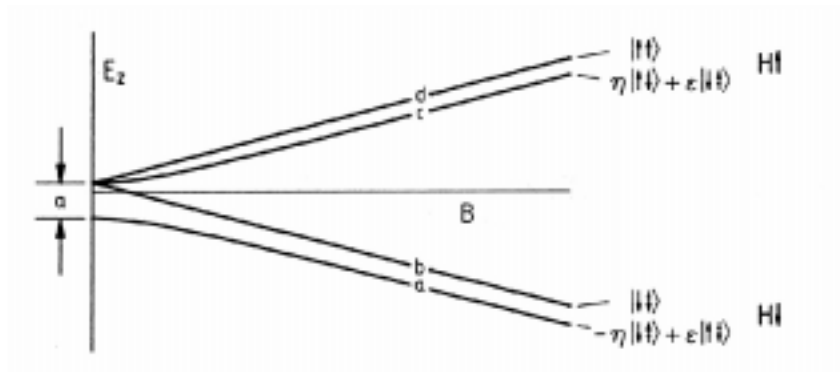


Figure 1.1: The hyperfine structure of the $1S$ manifold of the hydrogen atom. E_z is the Zeeman energy, $\eta = \cos \theta$ and $\varepsilon = \sin \theta$; the other symbols are defined in the text.

1.1 Single atom properties

Atomic hydrogen (H) is a bosonic atom composed of an electron tightly bound to a proton and having a $^2S_{1/2}$ electronic ground state. Due to the presence of nonzero nuclear spin the ground state has hyperfine structure. The electronic and nuclear magnetic moments follow from $\boldsymbol{\mu}_e = -g_e\mu_B\mathbf{s}$ and $\boldsymbol{\mu}_p = g_p\mu_N\mathbf{i}$, respectively, where μ_B is the Bohr magneton, μ_N the nuclear magneton and g_e, g_p are the associated g factors (defined as positive numbers). In terms of these quantities the gyromagnetic ratios are defined by $\gamma_e = g_e\mu_B/\hbar \approx 1.76 \times 10^{11}\text{s}^{-1}\text{T}^{-1}$ and $\gamma_p = g_p\mu_N/\hbar \approx 2.68 \times 10^8\text{s}^{-1}\text{T}^{-1}$, where $2\pi\hbar$ is the Planck constant. The Hamiltonian describing the ground state hyperfine structure is given by the expression

$$H = (g_e\mu_B\mathbf{s} - g_p\mu_N\mathbf{i}) \cdot \mathbf{B} + a_h\mathbf{i} \cdot \mathbf{s}, \quad (1.1)$$

where $a_h/(2\pi\hbar) \approx 1420$ MHz is the hyperfine interaction constant. The Hamiltonian (1.1) for $s = \frac{1}{2}$ and $i = \frac{1}{2}$ leads to the well known energy level diagram shown in Figure 1.1 with a zero-field hyperfine splitting equal to a_h [6]. In zero field $\mathbf{f} = \mathbf{i} + \mathbf{s}$ and m_f are good quantum numbers, whereas in high fields ($B \gg a_h/\mu_e \simeq 50.7$ mT) this holds for m_s, m_i and m_f .

By convention the ground state hyperfine levels are labeled a, b, c and d in order of increasing energy in small magnetic field. The c and d levels cross at $B = 16.7$ T. The b and d states are pure spin states, the a and c states are hyperfine-mixed linear combinations of the high field basis states $|m_s, m_i\rangle$:

$$\begin{aligned} |a\rangle &= \sin \theta |\uparrow \downarrow\rangle - \cos \theta |\downarrow \uparrow\rangle, & |b\rangle &= |\downarrow \downarrow\rangle \\ |c\rangle &= \cos \theta |\uparrow \downarrow\rangle + \sin \theta |\downarrow \uparrow\rangle, & |d\rangle &= |\uparrow \uparrow\rangle \end{aligned} \quad (1.2)$$

where $\tan 2\theta \equiv a_h/[\hbar(\gamma_e + \gamma_p)B]$. The simple arrows \uparrow and \downarrow refer to the magnetic quantum number of the electron spins and crossed arrows \uparrow and \downarrow to that of the proton spins.

The gas phase is characterised by the spin-polarisation of the constituent atoms. Unpolarised gas is referred to as H, up or down electron-spin-polarised gases as $\text{H}\uparrow$ and $\text{H}\downarrow$, respectively. Further, one distinguishes the doubly (both electron and proton spin) polarised gases, consisting predominantly of *b*-state ($\text{H}\downarrow\downarrow$) or *d*-state ($\text{H}\uparrow\uparrow$) atoms. Sometimes it is convenient to describe the atoms by the direction of the force caused by a magnetic field gradient. For this purpose the terminology high-field-seekers (for $\text{H}\downarrow$) and low-field-seekers (for $\text{H}\uparrow$) is used. The first experiments with spin-polarised hydrogen were done with $\text{H}\downarrow$ [7]. In these lectures hydrogen is used as an example to introduce the properties of ultra-cold atomic gases confined near the field minimum of magnetostatic traps. Therefore, the discussion will be restricted primarily to the low-field-seeking gas, $\text{H}\uparrow$.

1.2 Interatomic interactions

The interaction between two H atoms depends on their spin states. Thus, the four $1^2S_{1/2}$ hyperfine states give rise to 16 potential energy curves. However, for the collisional motion a description in terms of two potential curves is often sufficient. The dominant interaction is the Coulomb interaction, which is usually written in a spin-dependent form as the sum of a direct (V_D) and an exchange (J) contribution

$$H_{int} = V_D(r_{ij}) + J(r_{ij})\mathbf{s}_i \cdot \mathbf{s}_j, \quad (1.3)$$

where $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$ is the internuclear distance between atoms i and j at position \mathbf{r}_i and \mathbf{r}_j . The Hamiltonian (1.3) conserves the total spin $\mathbf{S} = \mathbf{s}_i + \mathbf{s}_j$ and gives rise to a singlet ($S = 0$) potential, $V_s = V_D + \frac{1}{4}J$, and a triplet ($S = 1$) potential, $V_t = V_D - \frac{3}{4}J$, which correspond, respectively, to the $X^1\Sigma_g^+$ and the $b^3\Sigma_u^+$ electronic states of the quasi-molecule. The exchange interaction $J = V_t - V_s$ vanishes exponentially with the interatomic distance. The $X^1\Sigma_g^+$ and the $b^3\Sigma_u^+$ states are known to high accuracy [8, 9]. Both $V_t(r)$ and $V_s(r)$ are shown schematically in Figure 1.2. The triplet potential has a very shallow attractive minimum, only 6.5 K deep, located at $r_{min} \approx 4.16 \text{ \AA}$. The zero crossing of this potential occurs at an interatomic distance $r_0 \approx 3.68 \text{ \AA}$ and is thus rather large for a small atom like H. A convenient fitting function for the triplet potential is presented in the literature [10].

For two H atoms in the ‘pure’ hyperfine *d* state (or similarly for two atoms in the *b* state) we have full spin polarisation and the atoms interact purely via the triplet potential. Collisions between two *c* state atoms cannot be described in terms of a pure triplet or singlet potential but involve a mixed state due to the asymptotic presence of the hyperfine interaction. Neglecting some triplet-singlet crossover near $r_{ij} = 5.8 \text{ \AA}$ (where $J(r_{ij}) \approx a_h$) the interaction (1.3) enables a fairly accurate description of hyperfine transitions due to ‘spin-exchange’. A full account using a coupled-channel approach has been given [11].

The next interaction to consider is the magnetic dipole-dipole interaction

$$H_{dip} = \frac{\mu_0}{4\pi r_{ij}^3} [\boldsymbol{\mu}_i \cdot \boldsymbol{\mu}_j - 3(\boldsymbol{\mu}_i \cdot \hat{\mathbf{r}}_{ij})(\boldsymbol{\mu}_j \cdot \hat{\mathbf{r}}_{ij})], \quad (1.4)$$

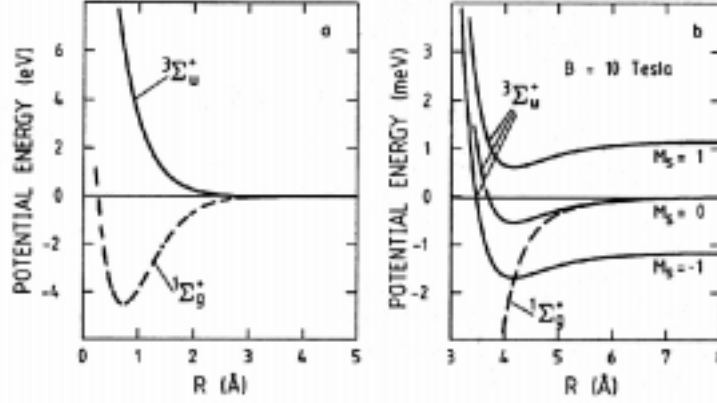


Figure 1.2: The singlet and triplet interatomic potentials as calculated by Kołos and Wolniewicz. Figure (b) shows the lifting of the electron-spin degeneracy by a magnetic field on a magnified scale with respect to Figure (a).

where $\boldsymbol{\mu}_i$ and $\boldsymbol{\mu}_j$ are the electronic spin-dipole moments of atoms i and j at relative position $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$, with modulus r_{ij} and direction unit vector $\hat{\mathbf{r}}_{ij}$. This interaction is responsible for the magnetic relaxation in d - d collisions and ultimately limits the stability of $\text{H}\uparrow$ in a magnetic trap. Note that the operator (1.4) does not induce triplet to singlet transitions as it conserves the total spin of the two interacting electrons (property of $s = 1/2$ system only!). The relaxation is associated with a change in total spin projection M_S which is possible because H_{dip} is a second rank tensor (in contrast to eqn. (1.3), which is isotropic) and therefore allows transfer of spin angular momentum to the orbital angular momentum of the atomic motion. For all interatomic distances relevant at low temperature the electron spin-dipole interaction is even weaker than the hyperfine interaction. To very good approximation the relaxation may be calculated in first order perturbation theory, using $V_t(r)$ to describe the relative atomic motion (distorted wave Born approximation). Spin-dipole interactions between an electron spin on one atom and a proton spin on the other atom are weaker by a factor γ_p/γ_e and unimportant in magnetostatic traps. The nuclear spin-dipole interaction is weaker by another factor γ_p/γ_e and is negligible in H for any practical purpose.

1.3 Stability considerations

In the context of the present paper we are mainly interested in the stability of the trappable, i.e., low-field-seeking gas, $\text{H}\uparrow$. A general treatment of the decay kinetics of atomic hydrogen, including two-body and three-body phenomena, was first given by Kagan *et al.* [12]. An introductory discussion is given in the review by Silvera and Walraven [3]. For magnetically trapped H the stability was analysed and calculated

in specialised papers (see [13, 11]). Here the discussion will be restricted to a brief summary.

The main causes for decay of $\text{H}\uparrow$ are spin exchange and magnetic dipolar interactions between the atoms. Spin exchange is most efficient (provided the hyperfine mixing angle is not too small) but only leads to relaxation in collisions between two c state atoms. For c - d collisions spin-exchange only proceeds via odd partial waves which are not populated at temperatures below 1 K (see section 2.2). Hence, in the case of d - d and c - d collisions, relaxation proceeds more slowly because it is induced by the relatively weak dipolar interaction. This implies a preferential depletion of the c -state component and ultimately leads to a pure d -state gas [13]. For a pure d -state sample the decay rate is given by the expression

$$\tau_{dip}^{-1} = n_0 \langle G_{dd} \rangle, \quad (1.5)$$

where $\langle G_{dd} \rangle$ is the loss rate constant for dipolar relaxation averaged over the trap. In the notation of Reference [11] the rate constant may be expressed as $G_{dd} = 2G_{ddaa}^d + G_{ddac}^d + G_{ddad}^d$. This notation shows the various contributions to the rate in terms of the detailed initial and final hyperfine states. Note that the relaxation events can produce atoms both in trapped and untrapped hyperfine states. Importantly, in the low temperature limit, $kT \ll a_h$, the dipolar rate constant (and thus also τ_{dip}^{-1}) is temperature independent. For the trap used in Amsterdam [14] with $n_0 = 10^{12} \text{ cm}^{-3}$ and $T = 10 \text{ mK}$ the average yields $\langle G_{dd} \rangle \approx 2 \times 10^{-15} \text{ cm}^3/\text{s}$ and $\tau_{dip} \approx 1000 \text{ s}$. For spin-exchange in a pure c -state gas under the same conditions one calculates $\langle G_{cc} \rangle \approx 10^{-13} \text{ cm}^3/\text{s}$ and $\tau_{ex} \approx 20 \text{ s}$. Here the rate constant may be expressed as $G_{cc} = 2G_{ccaa}^c + G_{ccac}^c + G_{ccbd}^c$. The dipolar relaxation rate has been measured both in Amsterdam [15] and at MIT [16]. The results are in agreement with theory. Thus far, the spin exchange rates have not been established experimentally in magnetic traps.

Unlike in other systems [17], such as the cold alkali vapors, three-body recombination is completely negligible in a pure d -state gas. This finds its origin in the extremely weak elastic potential that does not allow dimerisation. Three-body recombination in d -state hydrogen can only occur in combination with an electronic spin flip induced by the spin-dipole interaction [12].

Quantum gases

Let us now turn to a more general level and consider a thermal gas of cold atoms at number density n and temperature T . Assuming the atoms to interact pairwise via an isotropic central potential U the Hamiltonian has the following form

$$H = -\frac{\hbar^2}{2m} \sum_i \nabla_i^2 + \sum_{i<j} U(r_{ij}). \quad (2.1)$$

In such a gas the characteristic thermal momentum $\hbar k$ is given by $k \approx \Lambda^{-1}$, where $\Lambda \equiv [2\pi\hbar^2/(mk_B T)]^{1/2}$ is the thermal de Broglie wavelength ($\Lambda T^{1/2} \approx 17.4 \text{ \AA K}^{1/2}$ for H). If the temperature is sufficiently low, quantum mechanical effects determine the behaviour of the gas phase and the gas is referred to as a quantum gas. We raise the question ‘what makes a gas into a quantum gas?’ and analyse the difference between H and other experimentally investigated quantum gases, such as the optically cooled alkali systems or the metastable inert gases. Three quantum indicators will be analysed for this purpose. These are the zero-point motion of atoms (section 2.1), non-classical scattering in binary collisions (sections 2.2 and 2.3), and quantum degeneracy effects (section 2.4).

Before entering into this analysis, it should be emphasised that stable quantum gases do not exist. All stable substances condense into solid or liquid phases at temperatures approaching absolute zero. The quantum gases are therefore at best metastable, heavily oversaturated, vapors. Spin-polarised hydrogen is the only exception to this rule: it behaves at all temperatures as a fluid above its critical point. In this sense hydrogen is the only ‘true’ quantum gas. The metastability of spin-polarised hydrogen is therefore also of a different nature than that of other quantum gases. Because the spin-dipole interaction is so much weaker than the Van der Waals interaction, the spin-dipole induced recombination rate is very slow [12], 10 orders of magnitude slower than the dimerisation rate in caesium [17]. It is interesting to note here that, unlike the three-body processes such as dimerisation, two-body processes such as spin-dipole relaxation do not impose a fundamental limit on the densities that can be achieved in ultra-cold gases. Although the gas may survive longer at lower densities, it also takes longer to establish thermal (quasi-)equilibrium. The highest density that can be studied experimentally with hydrogen is therefore determined mostly by practical considerations such as the minimum time required to do a meaningful measurement. In

other quantum gases this density is limited by the dimerisation rate. In the following sections we take a practical attitude and address the properties of quantum gases as if these were stable. This means that we consider quantum gases on a time scale short as compared to their lifetime.

2.1 True quantum gases

The first quantum indicator that we consider is the importance of kinetic energy in substances at $T = 0$ K, i.e., the importance of zero-point motion. This is conveniently done within the quantum theory of corresponding states (QTCS) in which the Hamiltonian (2.1) is rewritten in the following dimensionless form [18, 19]

$$H = -\frac{1}{2}\eta \sum_i \nabla_i^{*2} + \sum_{i<j} u^*(r_{ij}^*), \quad (2.2)$$

where $\eta \equiv \hbar^2/m\epsilon r_0^2$ and

$$u^*(r_{ij}^*) \equiv U(r_{ij})/\epsilon \quad \text{with} \quad r_{ij}^* \equiv r_{ij}/r_0. \quad (2.3)$$

The QTCS applies to any class of systems that share an interaction potential of a given shape characterised by two parameters, one which sets the energy scale (ϵ) and the other the length scale (r_0). This holds, for instance, for all systems that may be described by a Lennard-Jones potential. Interestingly, the difference between the various systems in a given class (characterised by a potential of a given shape) appears exclusively through the quantum parameter η in front of the kinetic energy term of the Hamiltonian (2.2). The kinetic energy term gives rise to a positive contribution to the energy of the ground state, the potential energy contribution is negative except for very high densities where the repulsive cores dominate the interaction. For $\eta \rightarrow 0$ the kinetic energy is negligible and the ground state energy is minimal for conditions corresponding to a classical solid at its equilibrium density. With increasing η this solid will melt to form a quantum liquid. Further increasing η the ground-state energy will become positive at any density. This means that the liquid will become unbound: there is no many-body bound state. We are dealing with a true quantum gas that has to be confined by walls or in a trap to maintain constant density.

The ground-state energy of a many-body system described by Hamiltonian (2.1) is given by

$$E_0 = \langle \Psi | H | \Psi \rangle / \langle \Psi | \Psi \rangle, \quad (2.4)$$

where $|\Psi\rangle$ is the ground state. For the quantum liquids and gases E_0 has been calculated with variational wavefunctions of the Jastrow type, approximating the ground state of an N -body system by a product of $\frac{1}{2}N(N-1)$ pair wavefunctions $f(r_{ij})$

$$\Psi = F(r_1, \dots, r_N) \equiv \prod_{i<j} f(r_{ij}). \quad (2.5)$$

Then we have

$$\langle \Psi | H | \Psi \rangle = \sum_{i < j} \int \cdots \int F^2 \left[-\frac{\hbar^2}{2m} \nabla_i^2 \ln f(r_{ij}) + U(r_{ij}) \right] d\mathbf{r}_1 \cdots d\mathbf{r}_N. \quad (2.6)$$

This expression is obtained after integration by parts and repetitive use of the relation $\nabla_i F = F \sum_{j \neq i} \ln f(r_{ij})$. Introducing the pair correlation function

$$g(r) = \frac{N(N-1)}{n^2} \frac{\int \cdots \int \Psi^2 d\mathbf{r}_3 \cdots d\mathbf{r}_N}{\int \cdots \int \Psi^2 d\mathbf{r}_1 \cdots d\mathbf{r}_N}. \quad (2.7)$$

one obtains for the ground state energy *per atom*

$$E_0/N = \frac{1}{2}n \int g(r) \left[-\frac{\hbar^2}{2m} \nabla^2 \ln f(r) + U(r) \right] dr. \quad (2.8)$$

For a given choice for the Jastrow function $f(r)$, for example the form [20]

$$f(r) = \exp\left[-\frac{1}{2}(br_0/r)^5\right] \quad (2.9)$$

(with only a single variational parameter b), one can calculate $g(r)$ by a cluster expansion method [21] or a Monte Carlo procedure [22] and then find E_0/N by integration of Equation (2.8) and variation of the parameter b .

It was established [21] that Lennard-Jones Bose systems have a positive ground state energy for $\eta > 0.46$. Comparing the Lennard-Jones quantum parameters for various substances

	H	D	⁴ He	H ₂	Li	Na	Cs
η	0.55	0.275	0.18	8×10^{-2}	2×10^{-3}	5×10^{-4}	3×10^{-5}

shows that only spin-polarised hydrogen satisfies this condition. H is therefore the only substance that can remain gaseous under equilibrium conditions, i.e., the only true quantum gas. All other substances tend to form many-body bound states, usually crystalline solids. This may seem paradoxical in view of many practical experiments which have been done with the optically cooled alkali systems. At this point the metastability of all ultra-cold gases enters as an essential ingredient in the discussion and allows us to put the various systems in relative perspective. Although spin-polarised H has an intrinsically gaseous ground state, due to the presence of depolarisation mechanisms spin polarisation will never be complete and H is at best a metastable gas. Expanding the discussion to *metastable* systems in quasi-equilibrium it will follow from the next section that also systems with $\eta \ll 0.46$ can show gaseous behaviour as long as the formation of the many-body bound state can be excluded kinetically.

2.2 Quantum aspects in binary collisions

2.2.1 *s*-wave scattering regime

Let us leave many-body behaviour for a while and turn to quantum mechanical aspects of the relative motion of a pair of atoms under the influence of the interaction potential

U (V_t for spin-polarised H). The standard treatment involves partial waves of different angular momentum l (see for instance section 132 in [23])

$$\psi = \sum_l A_l P_l(\cos \theta) R_{kl}(r), \quad (2.10)$$

where the R_{kl} are wavefunctions satisfying the radial Schrödinger equation and the A_l are constants

$$[-d^2/dr^2 + l(l+1)/r^2 + \mathcal{V}(r) - k^2]rR_{kl}(r) = 0. \quad (2.11)$$

Here $\mathcal{V}(r) \equiv (m/\hbar^2)U(r)$, $k \equiv (mE/\hbar^2)^{1/2}$ is the wavenumber corresponding to the relative energy E and m (1.6735×10^{-27} kg for H) the mass of the atoms. For sufficiently large values of r the \mathcal{V} term may be neglected in Equation (2.11), which implies that the solutions always have the same asymptotic form $rR_{kl}(r) \sim \sin(kr - \frac{1}{2}l\pi + \eta_l)$ for $r \rightarrow \infty$. For $\mathcal{V}(r) \equiv 0$ the phase shifts η_l are identically zero, in any other case the η_l have to be evaluated explicitly. The amplitude $f(\theta)$ for scattering over an angle θ by the potential U is fully determined by the asymptotic behaviour of the wavefunction ψ and may therefore be expressed in terms of the η_l . Using the expansion

$$f(\theta) = \sum_l (2l+1) f_l P_l(\cos \theta), \quad (2.12)$$

the partial amplitudes f_l are related to the phases η_l by $f_l = (e^{2i\eta_l} - 1)/2ik$.

For $l > 0$ the third term of Equation (2.11) dominates over the (repulsive) second term only for distances $r < R_0$, where R_0 ($\sim 4.7 \text{ \AA}$ for spin-polarised H) is the range of the interaction (radius of action) defined by $R_0^2 = \mathcal{V}(R_0)$. This means that for

$$kR_0 \ll 1 \quad (2.13)$$

the \mathcal{V} term may be neglected in Equation (2.11) (for these k values the classical turning point R_{cl} for the radial motion is much larger than R_0). Therefore, all scattering has to result from the $l = 0$ channel. In the gas phase, where $k \approx \Lambda^{-1}$, the condition (2.13) is satisfied for

$$\Lambda \gg R_0. \quad (2.14)$$

The range of temperatures corresponding to condition (2.14) defines the s -wave scattering regime. For hydrogen this regimes covers temperatures $T \ll 1$ K. Under these conditions we are dealing with a pure quantum gas with only isotropic scattering through the s -wave channel.

For s -waves and for $k \rightarrow 0$ the phase shift is given by the following asymptotic expression

$$k \cot \eta_0(k) \simeq -\frac{1}{a} + \frac{1}{2}r_e k^2 \quad \text{for } k \rightarrow 0 \quad (2.15)$$

where a is the s -wave scattering length and r_e the effective range of interaction. For the V_t potential of hydrogen we have $a = 1.33 a_0$ and $r_e = 323 a_0$ (see [24, 25]). For $k \ll [\frac{1}{2}ar_e]^{-1/2}$ Equation (2.15) reduces to $\eta_0 \simeq -ka$. Note that this inequality hardly differs from condition (2.13) so that in the s -wave scattering regime the amplitude of scattering in any direction Ω becomes

$$f(\Omega) \approx f_0 = \frac{e^{i\eta_0}}{k} \sin \eta_0 \approx -a, \quad (2.16)$$

independent of both k and Ω . For bosons the differential cross section is given by the expression

$$d\sigma(\Omega) = |f(\Omega) + f(-\Omega)|^2 d\Omega = 4|f_0|^2 d\Omega. \quad (2.17)$$

Integrating over a hemisphere yields the total elastic cross section $\sigma = 8\pi a^2$ ($\sim 1.3 \times 10^{-15}$ cm² for spin-polarised H).

The formal expression for the l -wave amplitude of scattering in the direction Ω is given by

$$f_l(k, \Omega) = - \int j_l(kr) \mathcal{V}(r) R_{kl}(r) r^2 dr \quad (2.18)$$

where j_l is a spherical Bessel function (see for instance [26]). The asymptotic expression for R_{k0} coincides with the corresponding expression for s -wave scattering of hard spheres of diameter a :

$$R_{k0}(r) \simeq (kr)^{-1} \sin k(r - a) \approx 1 - a/r, \quad (kr \rightarrow 0, r \rightarrow \infty). \quad (2.19)$$

Hence the wavefunction equals unity everywhere except in a small region of radius R_0 around the scattering center.

2.2.2 Binary collision approximation

As long as the density is sufficiently low, the properties of gases may be described in terms of binary collisions with asymptotic wavefunctions of the type discussed above. Such gases are known as ‘nearly ideal gases’. This pair approximation is valid when collisions within the range of interaction with a third atom are of negligible importance, i.e., when the mean particle separation $n^{-1/3}$ is much larger than the range of the interaction

$$n^{1/3} R_0 \ll 1 \quad (2.20)$$

($n \ll 10^{20}$ cm⁻³ for spin-polarised H). More generally, if no other length scales of order R_0 or smaller have to be considered one may replace U by a point interaction, or pseudo potential

$$U(r) = v_0 \delta(\mathbf{r}) \quad \text{with} \quad v_0 \equiv (4\pi\hbar^2/m)a. \quad (2.21)$$

Note that by substituting Equation (2.21) into Equation (2.18), observing that $R_{k0}(r) = j_0(kr)$ in the absence of a phase shift, the scattering amplitude is found to be $-a$ as in Equation (2.16). The microscopic theory for nearly ideal Bose gases has been developed under the condition (2.20) using the quantity na^3 as a small parameter, the gas parameter [27]. For spin-polarised hydrogen we calculate $v_0 n/k_B \approx 40$ nK with $n = 10^{14}$ cm⁻³. Interestingly, as a tends to grow with growing mass, v_0 has, usually, more or less the same value.

2.3 Quantum statistical aspects

Large and heavy atoms, such as rubidium and caesium, can also form quantum gases, even though they fail to satisfy the corresponding states criterion mentioned in section 2.1. To understand why, one has to analyse how the quantum mechanical aspects

of binary collisions translate themselves in the properties of a gas. In the coming sections this will be done for s -wave Bose gases. It will be shown that the ground-state energy per atom, E_0/N , is (to leading order) linearly dependent on both the density of the atoms and their scattering length. Thus, in contrast to the corresponding states prediction for quantum gas behaviour, heavy atoms *with positive scattering length* can also satisfy the $E_0 > 0$ condition, i.e., behave as a quantum gas. The case of negative scattering length is special. Such systems want to lower their energy by contracting. This adds another level of metastability to the discussion which is not addressed further in this introductory context. Preference is given to showing that the interactions are experienced differently by ground-state atoms than by atoms in excited states of motion. All this assumes, of course, that the density fluctuations that give rise to triple, quadruple or higher order collisions can be neglected. This assumption is certainly true on time scales short as compared to the lifetime of the gas clouds.

2.3.1 Bose symmetrisation

Equation (2.21) represents a very powerful approximation for calculating many-body properties of low-density gases. Before turning for this purpose to a formal many-body description we first have a look how effects related to Bose symmetrisation come about.

For a pair of atoms the wavefunction is written as

$$\psi_{1,2} = \frac{1}{V} e^{-i\mathbf{k}_1 \cdot \mathbf{r}_1} e^{-i\mathbf{k}_2 \cdot \mathbf{r}_2} = \frac{1}{V} e^{-i\mathbf{K} \cdot \mathbf{R}} e^{-i\mathbf{k} \cdot \mathbf{r}}, \quad (2.22)$$

where $\mathbf{K} = \mathbf{k}_1 + \mathbf{k}_2$, $\mathbf{R} = \frac{1}{2}(\mathbf{r}_1 + \mathbf{r}_2)$ are the center of mass wavevector and position vector, respectively. Similarly $\mathbf{k} = \frac{1}{2}(\mathbf{k}_1 - \mathbf{k}_2)$, $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$ are the relative wavevector and position vector corresponding to the reduced mass. V is the normalisation volume. The expression (2.22) is ideal for mathematical manipulation but does not include the proper correlations at short distances. However, as long as we are not interested in properties that vary over a length scale of order R_0 , this objection may be circumvented by turning to the point interaction (2.21). Note further that the wavefunction (2.22) is not yet symmetrised. Both aspects will be considered here explicitly in calculating, to leading order in the density, the energy associated with the interaction potential V_l that gives rise to the elastic scattering in the gas. In the individual scattering events the direction of the relative momentum changes from \mathbf{k} to \mathbf{k}' ($|\mathbf{k}| = |\mathbf{k}'|$). The momentum transfer is $\mathbf{q} = \mathbf{k} - \mathbf{k}'$.

(a) We first consider the case $\mathbf{k}_1 = \mathbf{k}_2$. Then Equation (2.22) has the proper symmetrisation for bosons and with Equation (2.21) the perturbation matrix element of elastic interaction with momentum transfer \mathbf{q} is given by the following expression

$$\tilde{U}(q) = \frac{1}{V} \int^V v_0 \delta(\mathbf{r}) e^{i\mathbf{q} \cdot \mathbf{r}} d\mathbf{r}, \quad (2.23)$$

where the \mathbf{R} dependence has been integrated out. Because the relative momentum is zero ($\mathbf{k} = 0$) we also have $\mathbf{q} = 0$ (elastic scattering) and Equation (2.23) is easily integrated using to yield $\tilde{U}(0) = v_0/V$. We see that the elastic interaction energy is positive (i.e., effectively repulsive) for $a > 0$.

A particularly interesting special case is a gas of N bosons in a volume V with $\mathbf{k}_1 = \mathbf{k}_2 = \dots = \mathbf{k}_N = 0$ which corresponds to Bose condensed ideal gas at $T = 0$. With $\frac{1}{2}N(N-1) \approx \frac{1}{2}N^2$ pairs ($N \gg 1$) and assuming pair-wise interaction the total energy is $E_0 = \frac{1}{2}N^2\tilde{U}(0)$. The energy per atom is found to be

$$E_0/N = \frac{1}{2}nv_0. \quad (2.24)$$

(b) We now turn to the case $\mathbf{k}_1 \neq \mathbf{k}_2$. Then, Equation (2.22) has to be symmetrised while conserving normalisation. This leads to

$$\psi_{1,2} = \frac{1}{V}e^{-i\mathbf{K}\cdot\mathbf{R}}\frac{1}{\sqrt{2}}(e^{i\mathbf{k}\cdot\mathbf{r}} + e^{-i\mathbf{k}\cdot\mathbf{r}}) \quad (2.25)$$

and we obtain instead of Equation (2.23)

$$\tilde{u}(q, Q) = \frac{1}{V} \int^V v_0 \delta(\mathbf{r}) \frac{1}{2} [e^{i\mathbf{q}\cdot\mathbf{r}} + e^{i\mathbf{Q}\cdot\mathbf{r}} + e^{-i\mathbf{Q}\cdot\mathbf{r}} + e^{-i\mathbf{q}\cdot\mathbf{r}}] d\mathbf{r}, \quad (2.26)$$

where $\mathbf{Q} = \mathbf{k} + \mathbf{k}'$. Hence, we have $\tilde{u}(q, Q) \approx 2v_0/V$ provided the approximation (2.21) is valid ($kR_0, QR_0 \ll 1$). For a Bose condensed gas of N atoms with all except $N' \ll N$ in the condensate we find for the interaction energy per non-condensate atom

$$E'/N' = nv_0, \quad (2.27)$$

twice as big as Equation (2.24).

2.3.2 Many-body formalism

The differences in treatment between singly and multiply occupied states in many-body systems, as illustrated in the above example, are conveniently handled in the number representation (second quantisation). The peculiarities of Bose systems become here explicit through the definition of the number states, the construction operators and the commutation rules. The symmetrised many-body state $|\Psi\rangle = |n_1, n_2, \dots\rangle$ with n_i bosons in state $|i\rangle$ and $\sum_i n_i = N$ is given by

$$|n_1, n_2, \dots\rangle = \left(\frac{1}{N!n_1!n_2!\dots}\right)^{1/2} \sum_P |n_1, n_2, \dots\rangle, \quad (2.28)$$

where the sum runs over all possible permutations P of the unsymmetrised product states $|n_1, n_2, \dots\rangle$. In second quantisation, using field operators $\hat{\psi}^\dagger(\mathbf{r})$ and $\hat{\psi}(\mathbf{r})$, the potential energy operator has the following form (see for instance section 64 of [23])

$$\hat{U} = \frac{1}{2} \int \int d\mathbf{r}_1 d\mathbf{r}_2 \hat{\psi}^\dagger(\mathbf{r}_1) \hat{\psi}^\dagger(\mathbf{r}_2) U(\mathbf{r}_1 - \mathbf{r}_2) \hat{\psi}(\mathbf{r}_2) \hat{\psi}(\mathbf{r}_1) \quad (2.29)$$

which may be rewritten as

$$\hat{U} = \frac{1}{2} \int \int d\mathbf{r}_1 d\mathbf{r}_2 U(\mathbf{r}_1 - \mathbf{r}_2) \hat{g}(\mathbf{r}_1, \mathbf{r}_2), \quad (2.30)$$

where $\hat{g}(\mathbf{r}_1, \mathbf{r}_2) = \hat{\psi}^\dagger(\mathbf{r}_1)\hat{\psi}^\dagger(\mathbf{r}_2)\hat{\psi}(\mathbf{r}_2)\hat{\psi}(\mathbf{r}_1)$ is the correlation operator. Choosing a particular basis $\hat{\psi}^\dagger(\mathbf{r}) = \sum_k \varphi_k^*(\mathbf{r})a_k^\dagger$ the expectation value of \hat{g} becomes

$$g(\mathbf{r}_1, \mathbf{r}_2) = \sum_{klpq} \varphi_k^*(\mathbf{r}_1)\varphi_l^*(\mathbf{r}_2)\varphi_p(\mathbf{r}_2)\varphi_q(\mathbf{r}_1) \langle \Psi | a_k^\dagger a_l^\dagger a_p a_q | \Psi \rangle. \quad (2.31)$$

The only non-zero terms in the summation correspond to the combinations $k = p, l = q$ and $k = q, l = p$. Using the Bose commutation relations $[a_k, a_{k'}^\dagger] = \delta_{k,k'}$ we find for plane wave basis functions

$$g(\mathbf{r}_1 - \mathbf{r}_2) = \frac{1}{V^2} \sum_{k \neq l} (1 + e^{i(\mathbf{l}-\mathbf{k}) \cdot (\mathbf{r}_1 - \mathbf{r}_2)}) n_k n_l + \frac{1}{V^2} \sum_k n_k [n_k - 1]. \quad (2.32)$$

In a thermal gas typical values of wavevectors k, l are of order Λ^{-1} . Hence, for Equation (2.32) two regimes should be distinguished. Within the quantum correlation range, $|\mathbf{r}_1 - \mathbf{r}_2| \ll \Lambda$, the two-point correlation function g is twice as big as outside this range where the effect of the oscillating terms averages out. For the operator \hat{U} (2.30), representing the elastic interactions, this implies that at (low) temperatures where $\Lambda \gg R_0$, Bose correlations should be taken into account. Note that we arrived at the same conclusion in section 2.2, see Equation (2.14), in a different context. Equation (2.32) shows that the Bose correlations are present independent of the existence of any interaction.

Replacing U by a point interaction of the type (2.21) the operator \hat{U} can be expressed in terms of the operator density $\hat{\mathcal{Z}}(\mathbf{r}) = \hat{\psi}^\dagger(\mathbf{r})\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r})\hat{\psi}(\mathbf{r})$ that enables the determination of the interaction energy as a function of position, for example in inhomogeneous systems. By integrating over position the full operator \hat{U} is obtained,

$$\hat{U} = \frac{1}{2} v_0 \int d\mathbf{r} \hat{\mathcal{Z}}(\mathbf{r}). \quad (2.33)$$

Using the Bose commutation relations and retaining only those terms that yield a non-zero contribution to Equation (2.31) we find

$$\hat{\mathcal{Z}}(\mathbf{r}) = \sum_k |\varphi_k(\mathbf{r})|^4 \hat{n}_k [\hat{n}_k - 1] + 2 \sum_{k \neq l} |\varphi_k(\mathbf{r})|^2 |\varphi_l(\mathbf{r})|^2 \hat{n}_k \hat{n}_l. \quad (2.34)$$

Splitting-off the ground state explicitly

$$\hat{\psi}^\dagger(\mathbf{r}) = \hat{\psi}_0^\dagger(\mathbf{r}) + \hat{\psi}'^\dagger(\mathbf{r}) = \varphi_0^*(\mathbf{r})a_0^\dagger + \sum_{k \neq 0} \varphi_k^*(\mathbf{r})a_k^\dagger \quad (2.35)$$

we have

$$\hat{\mathcal{Z}}(\mathbf{r}) = |\varphi_0(\mathbf{r})|^4 \hat{n}_0 [\hat{n}_0 - 1] + 4\hat{n}_0(\mathbf{r}) \sum_{k \neq 0} \hat{n}_k(\mathbf{r}) + \hat{\mathcal{Z}}_{(k,l) \neq 0}(\mathbf{r}) \quad (2.36)$$

where $\hat{n}_k(\mathbf{r}) = |\varphi_k(\mathbf{r})|^2 \hat{n}_k$, with $\hat{n}_k = a_k^\dagger a_k$. Using $\sum_{k \neq 0} \hat{n}_k = \hat{n}' = \hat{N} - \hat{n}_0$ with $N_0 \gg n_k$ and retaining only terms of order n'^2 or larger we find

$$\langle U \rangle \approx v_0 \int d\mathbf{r} [\frac{1}{2} n_0^2(\mathbf{r}) + 2n_0(\mathbf{r})n'(\mathbf{r}) + n'^2(\mathbf{r})]. \quad (2.37)$$

Note by comparing the special cases $n_0 = 0$ and $n' = 0$ the difference of a factor 2 (at equal density) for the interaction energy per unit volume. This difference has the same origin as the difference between eqs. (2.24) and (2.27). It embodies a stabilising effect for the Bose condensate $n_0(\mathbf{r})$ at positive values of v_0 . For $v_0 < 0$ it points to a destabilising factor.

2.4 Quantum degeneracy in inhomogeneous Bose gases

The current interest in Bose gases mostly concerns the nearly ideal gas in the presence of an externally applied confining potential $\mathcal{U}(\mathbf{r})$. In relation to atomic hydrogen this problem was first addressed at the beginning of the last decade by Walraven and Silvera [28] and further investigated by Goldman *et al.* [29] and Huse and Siggia [30]. Later, after the first trapping proposals for hydrogen were published [31, 32] the topic was discussed by Lovelace and Tommila [33], Bagnato *et al.* [34] and in relation to stability considerations by Hijmans *et al.* [35]. Most recently dynamical aspects were investigated using time-dependent mean field solutions for the condensate [36]. All these authors considered quasi-homogeneous conditions as defined by the inequality

$$kT \gg nv_0 \gg \hbar\omega. \quad (2.38)$$

The low density case $nv_0 \ll \hbar\omega$, investigated in relation to the stability of gases with negative scattering length [37], is not considered in the present text.

It is the purpose of the coming sections to show that at temperatures above the critical temperature for Bose-Einstein condensation, T_c , the elastic interactions do not affect the density distribution of the gas to any appreciable extent (i.e., can be neglected), but that even slightly below T_c they are of major importance to determine the shape of the Bose condensate.

2.4.1 Ideal Bose gas in confining potential

To introduce the notation, first the case of an ideal Bose gas in an external potential is briefly summarised. The single particle eigenstates $\{\varphi_k(\mathbf{r})\}$, labeled by index k , with eigenvalues ε_k satisfy the following Schrödinger equation

$$\left\{-\frac{\hbar^2}{2m}\Delta + \mathcal{U}(\mathbf{r})\right\}\varphi_k(\mathbf{r}) = \varepsilon_k\varphi_k(\mathbf{r}). \quad (2.39)$$

With the grand ensemble the thermodynamic properties of the gas follow from the statistical operator

$$\hat{\rho}_0 = \exp[(-\Omega_0 + \mu\hat{N} - \hat{H}_0)/kT] = \frac{1}{Z_{gr}} \exp[(\mu\hat{N} - \hat{H}_0)/kT] \quad (2.40)$$

with normalisation $Tr\langle\hat{\rho}_0\rangle = 1$. Here Ω_0 is the thermodynamic potential (that normalises the trace of the density matrix), \hat{H}_0 is the Hamiltonian operator of the ideal

gas, μ is the chemical potential and \hat{N} is the number operator. The grand canonical partition function is defined by

$$Z_{gr} \equiv \exp[\Omega_0/kT] = Tr\langle \exp[(\mu\hat{N} - \hat{H}_0)/kT] \rangle. \quad (2.41)$$

The Hamiltonian \hat{H}_0 is diagonal in the number representation of the basis $\{\varphi_k(\mathbf{r})\}$

$$H_0(\mathbf{r}) = \sum_k \varepsilon_k |\varphi_k(\mathbf{r})|^2 Tr\langle \hat{\rho}_0 \hat{n}_k \rangle. \quad (2.42)$$

Evaluating the statistical average we find $Tr\langle \hat{\rho}_0 \hat{n}_k \rangle = \bar{n}_k$, where

$$\bar{n}_k = \frac{1}{\exp[(\varepsilon_k - \mu)/kT] - 1}. \quad (2.43)$$

The \bar{n}_k are the mean occupation numbers for the ideal Bose gas. By choosing the chemical potential such that $\sum_k \bar{n}_k = N$, the ensemble describes a trapped gas of N atoms at temperature T . At high temperatures μ has to be chosen large and negative. With decreasing temperature the chemical potential has to be chosen larger and larger until, at a finite temperature (T_c), it approaches ε_0 . Because expression (2.43) diverges for $\mu = \varepsilon_0$, the value of μ will never grow beyond ε_0 . An arbitrarily large ground state occupation is obtained by choosing μ sufficiently close to ε_0 . Therefore, below T_c , the value of μ is fixed and mean occupation numbers \bar{n}_k no longer depend on N but only on T . Their sum $\sum_{k \neq 0} \bar{n}_k = N'$ represents a finite number, vanishing with decreasing temperature. Hence, at T_c , the ground state occupation N_0 starts to become a macroscopic fraction of the total number of trapped atoms:

$$N_0 = N - \sum_{k \neq 0} \bar{n}_k. \quad (2.44)$$

This phenomenon, in which, at finite temperature, the statistics favours a macroscopic occupation of the ground state, is known as Bose-Einstein condensation (BEC).

Density distributions and BEC: For future reference it is useful to have a closer look at the density distribution $n(\mathbf{r})$ of a trapped Bose gas. With a large number of oscillator states occupied (quasi-homogeneous case) the ideal gas expression (2.43) may be approximated by a continuum expression for the distribution function

$$f(\varepsilon) = \frac{1}{z^{-1} \exp[-\varepsilon/kT] - 1} = \sum_{\ell=1}^{\infty} z^{\ell} \exp[-\ell\varepsilon/kT], \quad (2.45)$$

here also written as an expansion in terms of the fugacity $z = \exp[\mu/kT]$ (with $z < 1$ in the absence of a condensate), and normalised on the total number of trapped atoms

$$N = \int d\varepsilon \rho(\varepsilon) f(\varepsilon). \quad (2.46)$$

Here

$$\rho(\varepsilon) \equiv (2\pi\hbar)^{-3} \int d\mathbf{r} d\mathbf{p} \delta[\varepsilon - U(\mathbf{r}) - p^2/2m] \quad (2.47)$$

is the density of states in the quasi-classical phase space (\mathbf{r}, \mathbf{p}) . By changing to the continuum distribution we have implicitly set $\varepsilon_0 = 0$. Substituting eqs.(2.45) and (2.47) into Equation (2.46) and integrating over the momentum space we obtain

$$N = \frac{1}{\Lambda^3} \int d\mathbf{r} \sum_{\ell=1}^{\infty} \frac{z^\ell}{\ell^{3/2}} \exp[-\ell \mathcal{U}(\mathbf{r})/kT], \quad (2.48)$$

where Λ is the thermal wavelength. This expression fixes the value of the chemical potential for any given temperature. Writing $N = \int d\mathbf{r} n(\mathbf{r})$, we find for the density distribution

$$n(\mathbf{r}) = \frac{1}{\Lambda^3} g_{3/2}\{z \exp[-\mathcal{U}(\mathbf{r})/kT]\}. \quad (2.49)$$

Throughout this paper the usual notation $g_\alpha(x) \equiv \sum_{\ell=1}^{\infty} x^\ell / \ell^\alpha$ is used. For the center of a (deep) trap ($\mathbf{r} = 0$) Equation (2.49) can be written in the following form

$$n(0)\Lambda^3 = g_{3/2}(z). \quad (2.50)$$

This quantity is known as the degeneracy parameter of the trapped gas. Well above T_c we have the non-degenerate regime in which the degeneracy parameter is small, the fugacity expansion may be approximated by its first term, $g_{3/2}(z) \approx z$, and the chemical potential can be expressed as

$$\mu = kT \ln[n(0)\Lambda^3] \quad (2.51)$$

(note that μ is large and negative). At the onset of BEC the degeneracy parameter reaches its critical value, $n(0)\Lambda^3 = g_{3/2}(1) = 2.612$, and $\mu = 0$. Clearly, the critical density for BEC is first reached in the center of the trap. The degeneracy parameter is the same for any type of trap as long as the continuum approximation is valid and $\varepsilon_0 = 0$ [34].

The shape of the density distribution (2.49) changes with temperature. For $T \leq T_c$ it has a fixed form which, in the absence of an adjustable chemical potential μ , can only accommodate a fixed number of atoms

$$N' = \frac{1}{\Lambda^3} \int d\mathbf{r} g_{3/2}\{\exp[-\mathcal{U}(\mathbf{r})/kT]\} \quad (2.52)$$

(for any given temperature). Above T_c the distribution changes form until Equation (2.49) reaches its classical form,

$$n(\mathbf{r}) = n(0) \exp[-\mathcal{U}(\mathbf{r})/kT], \quad (2.53)$$

in the non-degenerate regime (i.e., for $z \lesssim 0.1$). For H at density $n = 10^{14} \text{ cm}^{-3}$ BEC occurs at $T_c \approx 30 \text{ } \mu\text{K}$. Note that for these numbers the conditions (2.14), (2.20) and the l.h.s. of Equation (2.38) are extremely well satisfied. Note further that at this density the mean free path, given by $\lambda \sim 1/n\sigma$, is of order 10 cm, much larger than the typical size of a trapped gas cloud.

Example: BEC in harmonic traps: It is instructive to consider BEC for the example a specific type of trap. For this purpose we first rewrite Equation (2.47) in the form

$$\rho(\varepsilon) = \frac{2\pi(2m)^{3/2}}{(2\pi\hbar)^3} \int_{\mathcal{U}(\mathbf{r}) \leq \varepsilon} d\mathbf{r} \sqrt{\varepsilon - \mathcal{U}(\mathbf{r})} \quad (2.54)$$

which implies that the density of states may be expressed as

$$\rho(\varepsilon) = A_{PL} \varepsilon^{1/2+\delta} \quad (2.55)$$

for square ($\delta = 0$), harmonic ($\delta = \frac{3}{2}$) and spherical-quadrupole ($\delta = 3$) traps, for spherically symmetric power-law traps with $\mathcal{U}(\mathbf{r}) \propto r^{3/\delta}$ and all power-law traps that may be written as $\mathcal{U}(x, y, z) \sim |x|^{1/\delta_1} + |y|^{1/\delta_2} + |z|^{1/\delta_3}$ with $\delta = \sum_i \delta_i$. In Equation (2.55) A_{PL} is a trap dependent constant.

For the case of an isotropic harmonic potential

$$\mathcal{U}(\mathbf{r}) = \frac{1}{2}m\omega^2 r^2, \quad (2.56)$$

where $r = |\mathbf{r}|$ and ω is the single atom oscillator frequency, we calculate

$$\rho(\varepsilon) = \frac{1}{2}(1/\hbar\omega)^3 \varepsilon^2. \quad (2.57)$$

For $T \leq T_c$ the fugacity equals unity and the number of above condensate particles is found by integration of Equation (2.46) using Equation (2.45) and substituting Equation (2.57) to yield $N' = (kT/\hbar\omega)^3 g_3(1)$. Thus, condensate fractions $N_0/N = 1 - N'/N$ close to unity are to be expected at temperatures even mildly below T_c . At T_c we have $N' = N_c$ and, therefore,

$$kT_c = (N/g_3(1))^{1/3} \hbar\omega \approx 0.941 N^{1/3} \hbar\omega. \quad (2.58)$$

Hence, to satisfy the inequality (2.38) appropriately at BEC, typically $N \gtrsim 10^6$ atoms are needed. With fewer atoms the quasi-homogeneous approximation starts to break down.

2.4.2 Nearly ideal Bose gas in a confining potential

In a nearly ideal Bose gas, i.e. if the gas parameter is small (see section 2.2.2), the analysis is done with a statistical variational method that leads to a mean field expression for the motion of the trapped atoms. Under condition (2.38) it follows with thermodynamic perturbation theory (see for instance [38]) that the thermodynamic potential Ω satisfies the following inequality

$$\Omega \leq \tilde{\Omega} = \Omega_0 + Tr \langle \hat{\rho}_0 (\hat{H} - \hat{H}_0) \rangle. \quad (2.59)$$

Here Ω_0 is the thermodynamic potential of the ideal Bose gas described by the Hamiltonian \hat{H}_0 which is used here as a trial Hamiltonian and $\hat{\rho}_0$ is the statistical operator of the

non-interacting gas defined by Equation (2.40). Choosing the number representation of the single particle basis $\{\varphi_k(\mathbf{r})\}$ we can derive using Equation (2.41)

$$\Omega_0(\mathbf{r}) = -kT \sum_k |\varphi_k(\mathbf{r})|^2 \ln[1 - e^{(\mu - \varepsilon_k)/kT}]. \quad (2.60)$$

Using operator densities, the full Hamiltonian is written as

$$\hat{H}(\mathbf{r}) = \hat{\psi}^\dagger(\mathbf{r}) \left\{ -\frac{\hbar^2}{2m} \Delta + \mathcal{U}(r) \right\} \hat{\psi}(\mathbf{r}) + \frac{1}{2} v_0 \hat{\mathcal{Z}}(\mathbf{r}). \quad (2.61)$$

Here approximation (2.21) was assumed to be valid. For inhomogeneous systems this requires the additional condition that interaction range should be much smaller than size of the oscillator ground state.

(a) No condensate ($T > T_c$).

We first consider the case of a weakly interacting gas without Bose condensate. In this case the energy density of the thermodynamic potential $\tilde{\Omega}(\mathbf{r})$ can be written as

$$\begin{aligned} \tilde{\Omega}(\mathbf{r}) &= \Omega_0(\mathbf{r}) + \sum_k \varphi_k^*(\mathbf{r}) \left\{ -\frac{\hbar^2}{2m} \Delta + \mathcal{U}(\mathbf{r}) - \varepsilon_k \right\} \varphi_k(\mathbf{r}) Tr \langle \hat{\rho}_0 \hat{n}_k \rangle + \\ &+ v_0 \sum_k |\varphi_k(\mathbf{r})|^4 \frac{1}{2} Tr \langle \hat{\rho}_0 \hat{n}_k [\hat{n}_k - 1] \rangle + \\ &+ v_0 \sum_{k \neq l} |\varphi_k(\mathbf{r})|^2 |\varphi_l(\mathbf{r})|^2 Tr \langle \hat{\rho}_0 \hat{n}_k \hat{n}_l \rangle \}. \end{aligned} \quad (2.62)$$

Evaluating the statistical averages we find $Tr \langle \hat{\rho}_0 \hat{n}_k \rangle = \bar{n}_k$, $Tr \langle \hat{\rho}_0 \hat{n}_k [\hat{n}_k - 1] \rangle = 2\bar{n}_k^2$ and $Tr \langle \hat{\rho}_0 \hat{n}_k \hat{n}_l \rangle = \bar{n}_k \bar{n}_l$, where the \bar{n}_k are the mean occupation numbers for the ideal Bose gas. For the interacting gas a better distribution function can be found by variation of the \bar{n}_k in order to minimize $\tilde{\Omega}(\mathbf{r})$:

$$\frac{\partial \tilde{\Omega}(\mathbf{r})}{\partial \bar{n}_k} = \varphi_k^*(\mathbf{r}) \left\{ -\frac{\hbar^2}{2m} \Delta + \mathcal{U}(\mathbf{r}) + 2v_0 \bar{n}(\mathbf{r}) - \varepsilon_k \right\} \varphi_k(\mathbf{r}). \quad (2.63)$$

The minimum is reached if $\partial \tilde{\Omega}(\mathbf{r}) / \partial \bar{n}_k = 0$ for all values of k simultaneously, i.e. if the following set of Hartree-Fock equations (coupled through the condition $n(\mathbf{r}) = \sum_k |\varphi_k(\mathbf{r})|^2 \bar{n}_k$) is satisfied

$$\left\{ -\frac{\hbar^2}{2m} \Delta + \mathcal{U}(\mathbf{r}) + 2v_0 n(\mathbf{r}) \right\} \varphi_k(\mathbf{r}) = \varepsilon_k \varphi_k(\mathbf{r}). \quad (2.64)$$

The eqs. (2.64) are known as the Ginzburg–Gross–Pitaevskii equations for an inhomogeneous Bose gas in the absence of a condensate [29, 30].

It is straightforward to show that the correction of $\mathcal{U}(\mathbf{r})$ by the mean field of the gas is negligible in the non-degenerate regime. For this we calculate the mean field correction to first order using the density distribution $n(\mathbf{r})$ of the ideal Bose given

by Equation (2.49). Expanding the potential energy terms in the Ginzburg-Gross-Pitaevskii equation around the origin

$$\mathcal{U}(\mathbf{r}) + 2v_0n(\mathbf{r}) = 2v_0n(0) + \frac{1}{2}m\omega^2r^2 \left[1 - \frac{g_{1/2}(z)}{g_{3/2}(z)} \frac{2v_0n(0)}{kT} + \dots \right]. \quad (2.65)$$

we find that the mean field correction consists of an energy shift $2v_0n(0)$ and a change of the spring constant of the oscillator of order $2v_0n(0)/kT$ which is very small in view of condition (2.38). Note that in the non-degenerate regime we have $g_{1/2}(z)/g_{3/2}(z) \approx 1$. Only very close to BEC, where the ratio $g_{1/2}(z)/g_{3/2}(z)$ diverges, the mean field correction to the spring constant may not be neglected and Equation (2.49) should be replaced by the self-consistent expression

$$n(\mathbf{r}) = \frac{1}{\Lambda^3} g_{3/2} \{ \exp[(\mu - 2v_0n(\mathbf{r}) - \mathcal{U}(\mathbf{r}))/kT] \}, \quad (2.66)$$

which is expected to be correct as long as the self-consistent potential varies sufficiently slowly that quasi-classical solutions to the Ginzburg-Gross-Pitaevskii equations are justified. The degeneracy parameter becomes in this case

$$n(0)\Lambda^3 = g_{3/2} \{ \exp[(\mu - 2v_0n(0))/kT] \} \quad (2.67)$$

and the onset of BEC, marked (as in the non-interacting case) by the condition $n(0)\Lambda^3 = g_{3/2}(1)$, occurs at

$$\mu = 2v_0n(0). \quad (2.68)$$

In terms of the total atom number the BEC criterion is given by the following self-consistent expression

$$N_c = \int d\mathbf{r} n(\mathbf{r}) = \frac{1}{\Lambda^3} \int d\mathbf{r} g_{3/2} \{ \exp[(2v_0n(0) - 2v_0n(\mathbf{r}) - \mathcal{U}(\mathbf{r}))/kT] \}, \quad (2.69)$$

which shows that, in comparison to ideal gases, repulsive Bose gases require more atoms to Bose condense at the same T_c .

(b) With condensate ($T < T_c$).

Below T_c we use the same variational procedure for $\tilde{\Omega}(\mathbf{r})$ but, since in the presence of a condensate we have $\mu = \varepsilon_0$ and $Tr\langle \hat{\rho}_0 \hat{n}_0 \rangle$ is diverging, we should single out the ground state from the ensemble average. We first single out the ground state in the Hamiltonian (2.61) using Equation (2.36) and setting $\langle \hat{n}_0 \rangle = N - \sum_{k \neq 0} Tr\langle \hat{\rho}_0 \hat{n}_k \rangle \equiv N_0$ and $\langle \hat{n}_0(\hat{n}_0 - 1) \rangle = N_0(N_0 - 1) \approx N_0^2$ (assuming $N_0 \gg 1$) before the ensemble average is evaluated in expression (2.62) for the thermodynamic potential. Variation with respect to \tilde{n}_k yields, for $k \neq 0$, the same result for $\partial\tilde{\Omega}(\mathbf{r})/\partial\tilde{n}_k$ as obtained above T_c , i.e., Equation (2.61) with $n(\mathbf{r}) = n_0(\mathbf{r}) + n'(\mathbf{r})$. Variation of N_0 gives rise to a different expression in which the exchange effects discussed in sections (2.3.1) and (2.3.2) again show up:

$$\frac{\partial\tilde{\Omega}(\mathbf{r})}{\partial N_0} = \varphi_0^*(\mathbf{r}) \left\{ -\frac{\hbar^2}{2m} \Delta + \mathcal{U}(\mathbf{r}) + v_0[n_0(\mathbf{r}) + 2n'(\mathbf{r})] - \mu \right\} \varphi_0(\mathbf{r}). \quad (2.70)$$

Consequently, below T_c we have the following set of Hartree-Fock equations

$$\left\{-\frac{\hbar^2}{2m}\Delta + \mathcal{U}(\mathbf{r}) + v_0[n_0(\mathbf{r}) + 2n'(\mathbf{r})]\right\}\varphi_0(\mathbf{r}) = \mu\varphi_0(\mathbf{r}) \quad (2.71)$$

$$\left\{-\frac{\hbar^2}{2m}\Delta + \mathcal{U}(\mathbf{r}) + 2v_0[n_0(\mathbf{r}) + n'(\mathbf{r})]\right\}\varphi_k(\mathbf{r}) = \varepsilon_k\varphi_k(\mathbf{r}) \quad (k \neq 0). \quad (2.72)$$

For $T \rightarrow 0$ the Equation (2.71) reduces to the Ginzburg-Gross-Pitaevskii equation for the many-body ground state [39, 40]. To find the expression for the chemical potential in the presence of a condensate we have to solve Equation (2.71). This is particularly simple for the quasi-homogeneous case since the condition $nv_0 \gg \hbar\omega$ enables us to neglect the kinetic energy term in Equation (2.71). Thus we find

$$\mu = \mathcal{U}(\mathbf{r}) + v_0[n_0(\mathbf{r}) + 2n'(\mathbf{r})] \quad (2.73)$$

and because μ should be constant over the sample we have

$$\mu = v_0[n_0(0) + 2n'(0)]. \quad (2.74)$$

Note that for $N_0 \rightarrow 0$ this equation reduces to Equation (2.68). Assuming the size of the condensate to be small as compared to the thermal size of the sample we may set $n'(\mathbf{r}) \approx n'(0)$ everywhere within the condensate and combine eqs. (2.73) and (2.74) to derive the following expression for the density distribution of the condensate

$$n_0(\mathbf{r}) = \frac{v_0 n_0(0) - \mathcal{U}(\mathbf{r})}{v_0} \quad (\text{for } |\mathbf{r}| \leq l_c). \quad (2.75)$$

For $|\mathbf{r}| \geq l_c$ we have $n_0(\mathbf{r}) \equiv 0$. The approximation $n'(\mathbf{r}) \approx n'(0)$ is readily verified for the example satisfied of the harmonic confining potential (2.56) where the $1/e$ thermal Gaussian width is given by $l_{th} = [2kT/m\omega^2]^{1/2}$. With Equation (2.75) the condensate radius is calculated to be $l_c = [2v_0 n_0(0)/m\omega^2]^{1/2}$. Thus with condition (2.38) it follows that $l_c \ll l_{th}$, i.e., the condensate manifests itself (also in the presence of interactions) as a spatially segregated high density phase in the center of the trapping potential. This is illustrated in fig.2.1.

Equation (2.75) presents a very important result for inhomogeneous Bose gases under quasi-homogeneous conditions. It shows that, for a given number (N_0) of atoms in the condensate, the density in the center of a condensate depends inversely on v_0 . In the absence of kinetic energy the condensate tends to be compressed by the confining potential. This leads to the divergence of the density in the case of an ideal gas. This unphysical divergence occurs because of the continuum approximation, which neglects the finite width of the oscillator ground state. The above analysis has shown that, below T_c , it is essential to include the repulsive interaction. Above T_c the presence of the interaction is much less important, actually almost negligible, because, under condition (2.38), the thermal motion counteracts the compression.

Figure 2.1 clearly shows one of the most fascinating and novel aspects of Bose condensates in inhomogeneous traps: The condensate appears as a small high-density

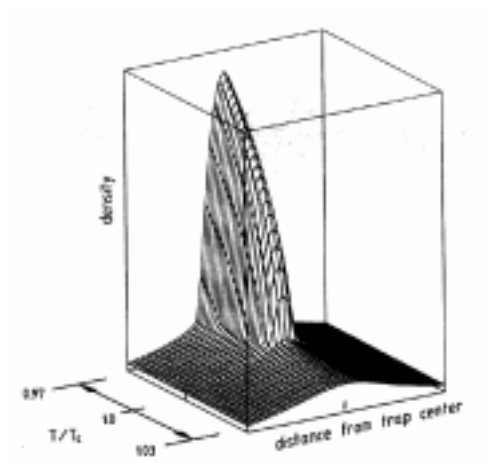


Figure 2.1: The density distribution for atomic hydrogen in the trap used in Amsterdam as a function of temperature near T_c . The condensate shows up as a sharp feature in the center of the distribution.

cloud of atoms in the center of the trapped gas and is, therefore, almost completely spatially separated from the non-condensate part. Thus we have the unique situation of a ground state surrounded by a cloud of excitations. It was shown in very recent BEC experiments with ^{87}Rb at JILA [5] that it is possible to remove this cloud of excitations rapidly while keeping the condensate. This implies cooling speeds which are limited primarily by the time required to remove the excited atoms and not by intrinsic properties such as the thermalisation time.

Evaporative cooling

3.1 Introduction

Evaporative cooling is a very powerful cooling method based on the preferential removal of atoms with an energy higher than the average energy per trapped atom and on thermalisation by elastic collisions. The evaporation process leads, under suitable conditions, to an increase in phase-space density, and was suggested for this purpose as a means to attain Bose-Einstein condensation (BEC) in atomic hydrogen [31, 41]. Presently, the method has been applied to a wider class of ultra-cold gases.

In this section the essential features of evaporative cooling will be discussed for Bose gases in the non-degenerate quantum regime. It will be assumed that the atoms are confined in a static potential well, $\mathcal{U}(\mathbf{r})$, from which they escape with unit probability as soon as their total energy, ε , exceeds a threshold value, ε_t , which is chosen to be much larger than the average energy per atom in the trap. As the most energetic atoms are removed in this way the gas will cool.

The basic assumption underlying the physical picture described above is ‘sufficient ergodicity’: It is assumed that the distribution of atoms in phase space (position and momentum) depends only on their energy. This will be the case, for example, in a trap with ergodic single-particle motion, in which case all parts of the equipotential hypersurface corresponding to the total energy of the atom are sampled with equal probability. However, as for many traps the single-particle motion is (partly) non-ergodic [42], interatomic collisions are usually essential to assure ‘sufficient ergodicity’.

In practical situations the escape can be arranged in various ways: by passing over a potential barrier [43, 44], by adsorbing onto a pumping surface [45, 46] or by optical [14] or RF [48, 49] pumping of the atoms to non-trapped states. If the evaporation is to be efficient it is essential that the escape occurs on a time scale short compared to the collisional time, i.e., that the mean free path λ is much larger than the size of the gas cloud l ,

$$\lambda \gg l. \tag{3.1}$$

One easily verifies that for H at density $n = 10^{14} \text{ cm}^{-3}$ (close to the highest density achieved in a trap), the mean free path, given by $\lambda \sim 1/n\sigma$, is of order 10 cm, indeed much larger than the typical size of a trapped sample. Spatial restrictions can limit the escape probability of energetic atoms and reduce the evaporative cooling power,

in particular in the case of non-ergodic single particle motion [42]. In this respect we discuss here ‘full-power evaporation’, evaporation limited only by the rate at which elastic collisions promote atoms to the escape energy.

Inevitably, the cooling of the gas will cause the evaporation process to slow down as fewer and fewer atoms can acquire the threshold energy. Eventually, the cooling rate is balanced by a competing heating mechanism or becomes negligibly small. The process just described will be referred to as ‘plain’ evaporative cooling, as opposed to ‘forced evaporative cooling’ where evaporation is forced to continue by lowering the escape threshold as the gas cools.

The principle of evaporative cooling was first demonstrated experimentally at MIT in the group of Greytak and Kleppner [50] who studied plain evaporative cooling by the escape of spin-polarised hydrogen atoms across a magnetic potential energy barrier. It was established, by measuring the quantity of gas remaining in the trap after a certain holding time, that this procedure causes the gas to cool to a temperature well below the temperature of the surrounding walls. The dynamics of this type of evaporative cooling was further studied optically [45, 46].

Forced evaporative cooling was also first applied to hydrogen [16, 51, 43, 44] and enabled temperatures as low as $100 \mu\text{K}$ and densities as high as $8 \times 10^{13} \text{cm}^{-3}$. This corresponds to $n\Lambda^3 \approx 0.4$, within one order of magnitude from the degenerate quantum regime. The need for sophisticated detection methods to establish density and temperature is limiting the progress towards lower temperatures here. An optical version of forced evaporative cooling of $\text{H}\uparrow$ was demonstrated in Amsterdam [14].

Recently, evaporative cooling methods were successfully applied to optically pre-cooled (and magnetically trapped) gases of sodium [48] and rubidium [49], both using RF-induced evaporation. In the final stage of preparation of the manuscript for the present paper BEC was announced for ^{87}Rb at JILA by the group of Cornell and Wieman [5] and by the group of Hulet at Rice University for ^7Li [52]. In both experiments evaporative cooling played a decisive role.

3.2 Truncated energy distributions

By its very nature (atoms in thermally accessible states are removed from the sample) evaporative cooling is an intrinsically non-equilibrium process in which a temperature, strictly speaking, cannot be defined. However, if the average energy per trapped atom is much smaller than the evaporation threshold, most interatomic collisions lead to a thermal redistribution of the energy over the trapped states. Thus, keeping in mind the discussion of section (2.4.2) (that, if the conditions $kT > kT_c \gg nv_0$ are satisfied, interaction effects are of minor importance) it is very appealing to assume that a quasi-equilibrium distribution will be established having the form (2.45), but with the tail of energies $\varepsilon > \varepsilon_t$ lacking:

$$f(\varepsilon) = \sum_{\ell=1}^{\infty} z^{\ell} \exp[-\ell\varepsilon/kT] \vartheta(\varepsilon_t - \varepsilon). \quad (3.2)$$

Here $\vartheta(x - x_0)$ is Heaviside's unit step function, zero for $x < x_0$ and unity for $x \geq x_0$. Such a distribution is characterised by three independent parameters: the truncation (escape) energy, ε_t , the quasi-temperature, T , and the degeneracy parameter, z . In the limit $\varepsilon_t \rightarrow \infty$, the parameters T and z reduce to the equilibrium temperature and fugacity, respectively. From Equation (3.2) it is clear that the truncation mostly affects the first term in the expansion. Being further aware that the thermodynamic properties are only mildly affected by degeneracy effects above the critical temperature for BEC, it is plausible that the essential aspects of evaporative cooling down to T_c can be obtained with the expression for the energy distribution of the non-degenerate regime

$$f(\varepsilon) = z e^{-\varepsilon/kT} \vartheta(\varepsilon_t - \varepsilon), \quad (3.3)$$

where z is determined by the normalisation condition (2.46) which becomes with (3.3)

$$N = z \int_0^{\varepsilon_t} d\varepsilon \rho(\varepsilon) e^{-\varepsilon/kT}. \quad (3.4)$$

Unlike (2.50), due to the truncation, the expression for the fugacity differs from the equilibrium expression (i.e., $z \neq n(0)\Lambda^3$). However, we can still formally write the degeneracy parameter as

$$z \equiv n_0 \Lambda^3, \quad (3.5)$$

choosing $\Lambda \equiv [2\pi\hbar^2/mkT]^{1/2}$ to coincide in the limit $\varepsilon_t \rightarrow \infty$ with the equilibrium expression for the thermal wavelength. With this procedure n_0 is a density, determined by the normalisation condition (3.4) and (only) coinciding in the limit $\varepsilon_t \rightarrow \infty$ with the density $n(0)$ in the trap center.

The truncated exponential form has been used as a starting point for several descriptions of evaporative cooling [53, 44, 47, 46]. It was shown by numerical solution of the Boltzmann equation [56], that for non-degenerate Bose gases the evaporation process, indeed, rather accurately conserves a quasi-equilibrium energy distribution of the form (3.2), a property noticed earlier in numerical simulations of evaporation experiments with trapped H at MIT [54].

One should be aware that the presence of the truncation edge affects all thermal properties. For example, to calculate the average thermal speed, the thermal wavelength, or the internal energy it is not sufficient to know the quasi-temperature (T), as these quantities also depend on the truncation energy (ε_t). In spite of this complication, once the truncated energy distribution (3.3) is adopted, a thermodynamic description of the sample follows naturally, with ε_t as one of the thermodynamic variables. In addition, the Boltzmann equation for the trapped gas can be radically simplified, allowing an explicit calculation of the rate of evaporation for different kinds of traps [56].

3.3 Thermodynamic properties

In this section we discuss a number of thermodynamic properties relevant for the description of evaporative cooling using the truncated exponential energy distribution (3.3) as a starting point. For the power-law traps defined in section (2.38) this can be

done very explicitly. In more general cases the classical canonical partition function of the truncated distribution turns out to be a central quantity. This can be seen directly from Equation (3.4), which can be rewritten as

$$N = n_0 \Lambda^3 \zeta \quad (3.6)$$

with

$$\zeta = \int_0^{\varepsilon_t} d\varepsilon \rho(\varepsilon) e^{-\varepsilon/kT}. \quad (3.7)$$

Substituting expression (2.47) for the density of states and introducing the classical single particle Hamiltonian, $H(\mathbf{r}, \mathbf{p}) = \mathcal{U}(\mathbf{r}) + p^2/2m$, we obtain

$$\zeta = (2\pi\hbar)^{-3} \int d\mathbf{p} d\mathbf{r} e^{-H(\mathbf{r}, \mathbf{p})/kT} \vartheta[\varepsilon_t - H(\mathbf{r}, \mathbf{p})], \quad (3.8)$$

which is the classical canonical partition function with the (truncated) region of phase space, $\mathcal{U}(\mathbf{r}) + p^2/2m \geq \varepsilon_t$, excluded.

3.3.1 Density distribution and effective volume

The density distribution $n(\mathbf{r})$ of the gas over the trap is obtained by evaluating, in Equation (3.6), only the momentum integral of the partition function and can be written as [55]

$$n(\mathbf{r}) = n_0 e^{-\mathcal{U}(\mathbf{r})/kT} P\left(\frac{3}{2}, \eta_t(\mathbf{r})\right), \quad (3.9)$$

where $P(a, \eta)$ is the incomplete gamma function (see appendix 3.5.4) and $\eta_t(\mathbf{r}) \equiv (\varepsilon_t - \mathcal{U}(\mathbf{r}))/kT$. Thus, for the truncated distribution, the true density in the trap center is given by

$$n(0) = n_0 P\left(\frac{3}{2}, \eta\right) \leq n_0, \quad (3.10)$$

where the parameter $\eta \equiv \eta_t(0) = \varepsilon_t/kT$ will be referred to as the truncation parameter and the (true) effective volume of the gas cloud is given by the expression

$$V_{eff} = N/n(0) = \int d\mathbf{r} n(\mathbf{r})/n(0). \quad (3.11)$$

Although the exact knowledge of V_{eff} is of practical importance, for example for the experimental determination of N , often it is more convenient to use a reference volume, V_e , defined in terms of the parameter n_0

$$V_e = N/n_0 = \Lambda^3 \zeta = \Lambda^3 \int_0^{\varepsilon_t} d\varepsilon \rho(\varepsilon) e^{-\varepsilon/kT}. \quad (3.12)$$

The volume V_e has very nice properties which result from its simple relation to the partition function. Moreover, since the degeneracy parameter for truncated distributions involves n_0 and not $n(0)$, see Equation (3.5), it may be better not to introduce $n(0)$ at all into the formalism.

Power-law traps: For the special case of a power-law trap the exponent δ , introduced in Equation (2.55), reappears in the expression for the partition function

$$\zeta = A_{PL} \int_0^{\varepsilon_t} d\varepsilon \varepsilon^{1/2+\delta} e^{-\varepsilon/kT} = \zeta_\infty P\left(\frac{3}{2} + \delta, \eta\right). \quad (3.13)$$

Here the limiting value, $\zeta_\infty = A_{PL}[kT]^{3/2+\delta}\Gamma(\frac{3}{2} + \delta)$, corresponds to an infinitely deep trap (i.e., $\eta \rightarrow \infty$) and $\Gamma(a)$ is the Euler gamma function. In particular, for (infinitely) deep harmonic traps, the partition function is given by $\zeta_\infty = \frac{1}{2} (kT/\hbar\omega)^3$.

The quasi-classical reference volume follows directly with Equation (3.12):

$$V_e = \Lambda^3 \zeta_\infty P(\frac{3}{2} + \delta, \eta). \quad (3.14)$$

Notice for deep power-law traps that they have a particularly simple temperature dependence of their reference volume,

$$V_e \propto T^\delta \quad \text{for } \eta \rightarrow \infty. \quad (3.15)$$

3.3.2 Internal energy

The internal energy (total energy) of a non-degenerate trapped gas of N atoms under (quasi-)equilibrium conditions is given by

$$E = n_0 \Lambda^3 \int_0^{\varepsilon_t} d\varepsilon \varepsilon \rho(\varepsilon) e^{-\varepsilon/kT}. \quad (3.16)$$

This expression can be rewritten in terms of the partition function (3.7)

$$E = NkT^2 \frac{1}{\zeta} \frac{\partial \zeta}{\partial T}, \quad (3.17)$$

a form, very well-known from statistical mechanics, that is seen to remain valid under quasi-equilibrium conditions in the trap. Substituting $\zeta = V_e/\Lambda^3$ it follows that

$$E = (\frac{3}{2} + \tilde{\gamma})NkT \quad (3.18)$$

where

$$\tilde{\gamma} \equiv \left(\frac{\partial \ln V_e}{\partial \ln T} \right)_{\varepsilon_t}. \quad (3.19)$$

The tilde symbol is used to remind us that the scaling parameter $\tilde{\gamma}$ depends on the truncation energy (ε_t) and further has a (slight) T dependence, $\tilde{\gamma} = \gamma(T, \varepsilon_t)$, due to the truncation or due to a density of states which deviates from the pure power-law density of states introduced in section 2.4.1. In cases where the momentum and position integrals in the partition function (3.8) can be separated, the terms $\frac{3}{2}NkT$ and $\tilde{\gamma}NkT$ in Equation (3.18) may be interpreted as kinetic and potential energy contributions to the total energy, respectively.

Note that Equation (3.18) remains valid also if the separation of momentum and position integrals is not possible. Therefore, it can serve as a good starting point for a general description of the quasi-equilibrium thermodynamic properties of trapped gases in terms of three independent variables: the total number of trapped atoms (N), the quasi-temperature (T) and the truncation energy (ε_t) or, equivalently, the truncation parameter (η). This description is the subject of section 3.5.

Power-law traps: For power-law traps it follows with eqs. (3.19) and (3.14) that the scaling parameter $\tilde{\gamma}$ depends only on the ratio of ε_t and T , i.e., on the truncation parameter (η),

$$\frac{3}{2} + \tilde{\gamma} = \left(\frac{3}{2} + \delta\right)R\left(\frac{3}{2} + \delta, \eta\right). \quad (3.20)$$

By definition $R(a, \eta) \equiv P(a + 1, \eta)/P(a, \eta)$, see further section 3.5.4. With Equation (3.20) the internal energy is found to be

$$E = E_\infty R\left(\frac{3}{2} + \delta, \eta\right), \quad (3.21)$$

where $E_\infty = \left(\frac{3}{2} + \delta\right)NkT$ is the internal energy of a sample of N atoms in thermal equilibrium in an infinitely deep trap. Note that the internal energy is independent of the details of the trap and depends only on the thermodynamic variables N, T and ε_t and on the scaling behaviour of the density of states (characterised for power-law traps by the δ parameter).

3.4 Kinetics of evaporation from a trap

Various questions arise from the intrinsic feature of particle loss in evaporative cooling. First of all one may have doubts about the efficiency of the cooling process. One may wonder whether there is any appreciable amount of sample left after it has been cooled to an interesting temperature or that the sample losses are excessive and disabling to the experimentalist. A related question concerns the choice of ε_t . It may be obvious that the extracted energy per evaporating atom is larger for larger ε_t but if this results in an impractically long cooling time the evaporation is of little use. Actually, what is meant by impractically long? Is this determined by the patience of the experimentalist, by instrumental limitations or by intrinsic properties of the gas? Starting from a kinetic equation, these and other questions and their relation to the shape of different traps will be discussed in the coming sections. Several characteristic parameters appear in this discussion: (a) the truncation parameter, $\eta \equiv \varepsilon_t/kT$, expressing the escape energy in terms of the quasi-temperature, (b) the ‘spilling’ parameters ξ , describing the scaling of the reference volume with ε_t and a measure for the spilling of atoms when ramping-down the escape threshold to force the evaporation and (c) the thermalisation ratio expressing the ratio of elastic collisions to loss collisions and thus determining whether or not thermal (quasi-)equilibrium can be established within the lifetime of the sample.

3.4.1 Kinetic equation

For a Bose gas in the s -wave regime and under sufficiently ergodic conditions (see section 3.1) the Boltzmann equation can be reduced to a kinetic equation for the distribution function $f(\varepsilon) = n_0\Lambda^3 \exp[-\varepsilon/kT]$ of a particularly simple form [56].

$$\rho(\varepsilon_4)\dot{f}(\varepsilon_4) = \frac{m\sigma}{\pi^2\hbar^3} \int d\varepsilon_1 d\varepsilon_2 d\varepsilon_3 \delta[\varepsilon_1 + \varepsilon_2 - \varepsilon_3 - \varepsilon_4] \times \quad (3.22)$$

$$\rho(\min[\varepsilon_1, \varepsilon_2, \varepsilon_3, \varepsilon_4])\{f(\varepsilon_1)f(\varepsilon_2) - f(\varepsilon_3)f(\varepsilon_4)\}.$$

This equation represents the detailed balance between collisions in which atoms with energy ε_1 and ε_2 produce atoms with energy ε_4 (under conservation of energy and momentum) and collisions in which atoms with energy ε_4 are lost from the distribution while producing atoms with energy ε_1 and ε_2 (conserving energy and momentum). Equation (3.22) describes the time evolution of the energy distribution function $f(\varepsilon)$ as a result of the elementary collisional processes: s -wave collisions with cross section $\sigma = 8\pi a^2$ (see section 2.2). Notably, this expression only involves the density of states of the atom with the lowest energy involved in each collisional process. This property was first used in the BEC literature to describe the kinetics of Bose condensation in homogeneous systems in relation to excitons [57] and in spin-polarised hydrogen [58, 59].

Equation (3.22) was derived for inhomogeneous systems to calculate the rate of evaporation from a trap (see section 3.4.2) and to study, by numerical solution, the time evolution of the shape of the truncated energy distribution [56]. In this way the use of the quasi-equilibrium approximation (3.3) could be justified.

3.4.2 Evaporation rate

By definition, the evaporation rate equals the rate of loss of atoms to non-trapped states ($\varepsilon_4 > \varepsilon_t$) as a result of collisions between trapped atoms, and is thus given by the following expression

$$\dot{N}_{ev} = - \int_{\varepsilon_t}^{\infty} d\varepsilon_4 \rho(\varepsilon_4) \dot{f}(\varepsilon_4). \quad (3.23)$$

In the truncated Boltzmann approximation we see that if $\varepsilon_4 > \varepsilon_t > \varepsilon_1, \varepsilon_2$ only the gain term in the kinetic equation (3.22) contributes and that $\varepsilon_3 = \varepsilon_1 + \varepsilon_2 - \varepsilon_4$ is necessarily the lowest energy involved in any collision involving escape of one of the atoms. Hence,

$$\dot{N}_{ev} = - \frac{m\sigma}{\pi^2 \hbar^3} \int_0^{\varepsilon_t} d\varepsilon_3 \int_{\varepsilon_3}^{\varepsilon_t} d\varepsilon_2 \int_{\varepsilon_3 + \varepsilon_t - \varepsilon_2}^{\varepsilon_t} d\varepsilon_1 \rho(\varepsilon_3) f(\varepsilon_1) f(\varepsilon_2) \quad (3.24)$$

where the domain of integration is determined by the requirements that $\varepsilon_1, \varepsilon_2 < \varepsilon_t$ and $\varepsilon_1 + \varepsilon_2 - \varepsilon_3 = \varepsilon_4 > \varepsilon_t$. Evaluating the integral is straightforward and yields

$$\dot{N}_{ev} = -n_0^2 \bar{v} \sigma e^{-\eta} V_{ev} \quad (3.25)$$

with $\bar{v} \equiv [8kT/\pi m]^{1/2}$ defined to coincide in the limit $\eta \rightarrow \infty$ with the equilibrium expression for the mean thermal speed, and V_{ev} is the reference volume for evaporation defined by

$$V_{ev} = \frac{\Lambda^3}{kT} \int_0^{\varepsilon_t} d\varepsilon \rho(\varepsilon) [(\varepsilon_t - \varepsilon - kT)e^{-\varepsilon/kT} + kTe^{-\varepsilon_t/kT}]. \quad (3.26)$$

Hence, the characteristic evaporational decay time τ_{ev} , defined by the expression $\tau_{ev}^{-1} = -\dot{N}_{ev}/N$, can be written as

$$\tau_{ev}^{-1} = n_0 \bar{v} \sigma e^{-\eta} V_{ev}/V_e. \quad (3.27)$$

Here it was used that all atoms that acquire, as a result of an elastic interatomic collision, an energy satisfying the evaporation condition ($\varepsilon_4 > \varepsilon_t$) are lost from the

trap with unit probability. The volume ratio V_{ev}/V_e can vary between zero and infinity and may be calculated numerically for any type of trap once the density of states is known. Note that the eqs. (3.25) and (3.27) hold for given values of N, T and ε_t . Clearly, for a proper description of evaporative cooling of a trapped cloud of gas we have to bring into the picture how the evaporation process affects N and T for fixed (plain evaporation) or time-varying (forced evaporation) value of the truncation parameter ε_t . We return to this point in section 3.5.

Equation (3.27) can be interpreted as a collision rate multiplied by an escape probability. However, the usual discussion associated with such an interpretation, concerning the influence of the thermalisation rate on the escape probability, is avoided by deriving expressions directly from the Boltzmann equation. All limitations with regard to the validity of Equation (3.27) are contained in the limitations to validity of the quasi-equilibrium approximation (3.3) and these limitations are known to be small for the quasi-homogeneous non-degenerate Bose gas discussed here [56].

Power-law traps: For these traps (introduced in section 2.4.1) the ratio V_{ev}/V_e can be expressed analytically in terms of incomplete gamma functions

$$V_{ev}/V_e = \eta - \left(\frac{5}{2} + \delta\right) R\left(\frac{3}{2} + \delta, \eta\right). \quad (3.28)$$

Taking notice of the asymptotic behaviour of the volume ratio

$$V_{ev}/V_e \simeq \frac{\eta^2}{\left(\frac{5}{2} + \delta\right)\left(\frac{3}{2} + \delta\right)} \quad (\eta \rightarrow 0) \quad \text{and} \quad V_{ev}/V_e \simeq \eta - \frac{5}{2} - \delta \quad (\eta \rightarrow \infty) \quad (3.29)$$

one may say, somewhat handwaving, that in many practical cases the assumption $V_{ev}/V_e \approx 1$ is not a bad approximation to estimate the order of magnitude of the evaporation rate.

3.4.3 Forced evaporation

Thus far ε_t was assumed to be constant, i.e., we only considered plain evaporation. In forced evaporation the escape threshold is slowly lowered in order to have the evaporation proceed at the desired rate. The evaporation process is very sensitive for the value of the truncation parameter (η) because it appears in the exponent of the expressions (3.25) and (3.27). Inevitably, the lowering of ε_t gives rise to an additional loss, not related to collision induced escape (evaporation), but to the change in escape condition itself. Therefore, in forced evaporation, the loss of atoms from the trap consists of two contributions,

$$\dot{N} = \dot{N}_{ev} + \dot{N}_t. \quad (3.30)$$

The first term is the evaporation loss rate discussed in the previous section. The second term is the truncation loss rate, only non-zero for $d\varepsilon_t/dt < 0$,

$$\dot{N}_t = \rho(\varepsilon_t) f(\varepsilon_t) \dot{\varepsilon}_t. \quad (3.31)$$

Rewriting in terms of the partition function, $\rho(\varepsilon_t)e^{-\eta} = (\partial\zeta/\partial\varepsilon_t)_T$, and substituting the expression $\zeta = V_e/\Lambda^3$ we obtain

$$\dot{N}_t/N = \tilde{\xi} \dot{\varepsilon}_t/\varepsilon_t, \quad (3.32)$$

where the scaling parameter $\tilde{\xi}$ is defined by

$$\tilde{\xi} \equiv \left(\frac{\partial \ln V_e}{\partial \ln \varepsilon_t} \right)_T. \quad (3.33)$$

Note that $\tilde{\xi} \approx 0$ for deep traps. Equation (3.32) expresses the relation between the characteristic time for atom loss due to truncation (τ_t), defined by the expression $\tau_t^{-1} = -(\dot{N}_t/N)$, and the ramp-down time (τ_{ramp}), defined by $\tau_{ramp}^{-1} = -(\dot{\varepsilon}_t/\varepsilon_t)$ and is easily rewritten for this purpose as $\tau_t^{-1} = \tilde{\xi} \tau_{ramp}^{-1}$. Hence, $\tilde{\xi}$ is a measure for the spilling of particles by the ramping procedure.

The overall decay time of the sample due to forced evaporation (τ) can be written as the sum of two terms,

$$\tau^{-1} = \tau_{ev}^{-1} + \tau_t^{-1}, \quad (3.34)$$

representing the rates of evaporation and truncation, respectively. In view of this result, we may distinguish two regimes:

- *Quasi-static ramping* ($\tau_t^{-1} \ll \tau_{ev}^{-1}$). In this regime the evaporation threshold ε_t is ‘slowly’ reduced and the atom loss is mainly due to evaporation. This is the regime of ‘pure’ forced evaporative cooling ($\dot{N} \approx \dot{N}_{ev}$) in which both N and T change. In the limit $\tau_t^{-1} \rightarrow 0$ we have plain evaporation.
- *Fast ramping (filtering)* ($\tau_t^{-1} \gg \tau_{ev}^{-1}$). In this regime essentially all particle loss is due to the truncation ($\dot{N} \approx \dot{N}_t$). The quasi-temperature remains *constant* but the internal energy, E , is reduced as the most energetic atoms are filtered from the sample (see next section).

Power-law traps: Rewriting Equation (3.33) for power-law traps we obtain

$$\tilde{\xi} = \left(\frac{3}{2} + \delta\right) [1 - R(\frac{3}{2} + \delta, \eta)]. \quad (3.35)$$

It is noteworthy that, for power-law traps, the sum of the two partial derivatives of the reference volume V_e reduces to a particularly simple form,

$$\tilde{\gamma} + \tilde{\xi} = \delta. \quad (3.36)$$

For the special case of harmonic traps the condition for quasi-static ramping may be expressed by an inequality for the product of the trap frequency (ω) and the ramp-down time (τ_{ramp}) in terms of three characteristic ratios, the truncation parameter, the ratio of quasi-thermal wavelength to the s -wave scattering length and the ratio of the quasi-temperature and level splitting

$$\omega \tau_{ramp} \gg \frac{1}{N} \left(\frac{\Lambda}{a} \right)^2 \left(\frac{kT}{\hbar\omega} \right)^2 \frac{\eta^3}{[\eta - 4R(3, \eta)]}. \quad (3.37)$$

3.4.4 Loss of internal energy

The rate at which the internal energy of the trapped gas decreases during the evaporation process is composed of two contributions,

$$\dot{E} = \dot{E}_{ev} + \dot{E}_t. \quad (3.38)$$

The first contribution (\dot{E}_{ev}) is the evaporation term, resulting from the interatomic collisions and representing the energy removed with the evaporating atoms. The second term (\dot{E}_t) gives the contribution due to a changing truncation energy, only present for $d\varepsilon_t/dt < 0$. In plain evaporation only the term \dot{E}_{ev} contributes. If ε_t is varied the truncation losses are given the following expression

$$\dot{E}_t = \varepsilon_t \rho(\varepsilon_t) f(\varepsilon_t) \dot{\varepsilon}_t = \varepsilon_t \dot{N}_t. \quad (3.39)$$

The internal energy loss due to evaporation follows from evaluation of the following integral

$$\dot{E}_{ev} = - \int_{\varepsilon_t}^{\infty} d\varepsilon_4 \varepsilon_4 \rho(\varepsilon_4) \dot{f}(\varepsilon_4). \quad (3.40)$$

With the same procedure as used in the previous section for calculating the evaporation rate (\dot{N}_{ev}), see Equation (3.25), we find

$$\dot{E}_{ev} = \dot{N}_{ev} [\varepsilon_t + (1 - X_{ev}/V_{ev}) kT], \quad (3.41)$$

where

$$X_{ev} = \frac{\Lambda^3}{kT} \int_0^{\varepsilon_t} d\varepsilon \rho(\varepsilon) [kT e^{-\varepsilon/kT} - (\varepsilon_t - \varepsilon + kT) e^{-\varepsilon_t/kT}]. \quad (3.42)$$

The volume ratio X_{ev}/V_{ev} can vary between zero and unity and is easily calculated numerically for arbitrary traps once the density of states is known. Like eqs. (3.25) and (3.27) also Equation (3.41) is valid for given N, T and ε_t . Equation (3.41) expresses the physical picture that atoms escaping from the trap reduce the internal energy by an amount slightly larger than the energy of the truncation edge ε_t .

Power-law traps: For these traps (see section 2.4.1) the ratio X_{ev}/V_{ev} can be expressed as

$$\frac{X_{ev}}{V_{ev}} = \frac{P(\frac{7}{2} + \delta, \eta)}{P(\frac{3}{2} + \delta, \eta)} \frac{V_e}{V_{ev}} \quad (3.43)$$

and the asymptotic behaviour is given by

$$X_{ev}/V_{ev} \simeq 1 - \frac{\eta}{\frac{9}{2} + \delta} \quad (\eta \rightarrow 0) \quad \text{and} \quad X_{ev}/V_{ev} \simeq \frac{1}{\eta - \frac{5}{2} - \delta} \quad (\eta \rightarrow \infty). \quad (3.44)$$

3.4.5 Relaxation heating and the thermalisation ratio

Just like evaporation leads to cooling because only the most energetic atoms escape, magnetic relaxation will lead to heating because in this process the low-energy atoms are preferentially removed. Because spin relaxation is a two-body process (see section 1.3)

the relaxation rate is proportional to the square of the gas density. Thus, the atoms are lost preferentially from the central region of the trap (region of highest density) where the atoms have lower-than-average energy. We assume here that *all* relaxation products leave the trapped gas: high-field-seeking atoms are ejected from the trap in accordance with their nature and the atoms in ‘trapped’ spin states because the recoil that accompanies (inelastic) relaxation events makes the atoms too energetic to be confined in the trap.

The rate of change of the number of trapped atoms due to spin relaxation can be written as

$$\dot{N}_{rel} = - \int d^3r G(\mathbf{r}) n^2(\mathbf{r}) \quad (3.45)$$

where the rate constant G is assumed to be independent of temperature (low temperature limit). Neglecting a possible position dependence (e.g. field dependence) of the rate constant and defining a characteristic relaxation time τ_{rel} by $\tau_{rel}^{-1} = -(\dot{N}_{rel}/N)$, Equation (3.45) can be reexpressed as

$$\tau_{rel}^{-1} = n_0 G V_{2e} / V_e, \quad (3.46)$$

where the reference volume for binary collisions is given by

$$V_{2e} = \int d^3r [n(\mathbf{r})/n_0]^2. \quad (3.47)$$

The associated rate of change of internal energy,

$$\dot{E}_{rel} = \dot{N}_{rel} \left(\frac{3}{2} + \tilde{\gamma}_2 \right) kT \quad (3.48)$$

where $\tilde{\gamma}_2 = [T/(2V_{2e})] \partial V_{2e} / \partial T$ is the scaling parameter for the collision reference volume. One may show that $\tilde{\gamma}_2 < \tilde{\gamma}$. Therefore, the relaxation effectively acts as a heating mechanism.

As both relaxation and evaporation are two-body processes their density dependence is identical. This allows us to combine eqs. (3.41) and (3.48) into a single expression for the energy loss rate,

$$\dot{E}_{ev} + \dot{E}_{rel} = \dot{N}_{ev} [\eta + (1 - X_{ev}/V_{ev}) + (\frac{3}{2} + \tilde{\gamma}_2)/\mathcal{R}] kT, \quad (3.49)$$

where \mathcal{R} is the thermalisation ratio (the ‘ratio of good-to-bad collisions’), defined by the expression $\mathcal{R} = \dot{N}_{ev}/\dot{N}_{rel}$. Substituting eqs. (3.27) and (3.46) the thermalisation ratio can be written as

$$\mathcal{R} = \frac{\bar{v}\sigma}{G} \frac{V_{ev}}{V_{2e}} e^{-\eta}, \quad (3.50)$$

notably independent of n_0 . Similarly one can write one combined expression for the atom loss rate due to binary collisional processes

$$\dot{N}_{ev} + \dot{N}_{rel} = \dot{N}_{ev} [1 + 1/\mathcal{R}]. \quad (3.51)$$

Since the elastic collision rate scales with $T^{1/2}$ whereas G is temperature independent (at low temperature) the thermalisation ratio decreases with decreasing temperature according to $\mathcal{R} \propto T^{1/2}$. Therefore, it is also useful to define a characteristic

temperature T_* at which an atom has equal probability to experience an inelastic or an elastic collision (in a full thermal distribution):

$$kT_* = \frac{\pi m G^2}{16\sigma^2}. \quad (3.52)$$

For hydrogen the thermalisation ratio is anomalously small as a result of the small s -wave cross section. Substituting the values for $\text{H}\uparrow$ in low magnetic fields one calculates $T_* \simeq 1.4 \text{ nK}$.

In many practical cases the thermalisation ratio will be large, $\mathcal{R} \gg \frac{3}{2} + \tilde{\gamma}_2$, so that the relaxation corrections may be neglected in eqs. (3.49) and (3.51). In view of this, the author has chosen not to contaminate the equations in the coming sections with these straightforward corrections, discussing the physics as if relaxation is absent.

3.5 Thermodynamics of evaporative cooling

With expressions for the particle loss and energy loss at our disposal we can return to the thermodynamical aspects and calculate the change of density (n_0) and the rate of cooling \dot{T}/T of the evaporating gas cloud. Two new scaling parameters will be introduced for this purpose. The efficiency parameter, $\tilde{\alpha}$, relates the quasi-temperature to the number of atoms remaining in the trap after a certain evaporation time, $T \propto N^{\tilde{\alpha}}$. The scaling parameter $\tilde{\beta}$ expresses how the density n_0 changes with quasi-temperature during cooling.

3.5.1 Plain evaporative cooling

We first consider the case of plain evaporative cooling. It is seen from eqs. (3.17) and (3.7) that, for a given trap, the internal energy only depends on three independent variables N , T and ε_t . Therefore, during any change of state in which these variables remain well defined, the internal energy change may be described by

$$dE = C_{\varepsilon_t} dT + \mu_{\varepsilon_t} dN + W_{\varepsilon_t} d\varepsilon_t, \quad (3.53)$$

where $C_{\varepsilon_t} = (\partial E / \partial T)_{N, \varepsilon_t}$ is the heat capacity at constant escape energy and for a fixed number of trapped atoms, $\mu_{\varepsilon_t} = (\partial E / \partial N)_{T, \varepsilon_t}$ is like a ‘chemical potential’ of evaporation at constant escape energy and $W_{\varepsilon_t} = (\partial E / \partial \varepsilon_t)_{N, T}$ is a heat of truncation at constant quasi-temperature and for a fixed number of atoms. With Equation (3.18) it follows immediately that

$$C_{\varepsilon_t} = \left(\frac{3}{2} + \tilde{\gamma} + T(\partial \tilde{\gamma} / \partial T)_{\varepsilon_t}\right) Nk \quad \text{and} \quad \mu_{\varepsilon_t} = \left(\frac{3}{2} + \tilde{\gamma}\right) kT. \quad (3.54)$$

This shows that μ_{ε_t} is nothing else than the average energy per remaining atom during evaporation, $\mu_{\varepsilon_t} \equiv E/N$.

For plain evaporative cooling, i.e., evaporative cooling at constant escape energy ε_t , the third term in Equation (3.53) does not contribute to the internal energy change, leaving only two independent thermodynamic variables, N and T .

Power-law traps: In this case the heat capacity at constant escape energy becomes

$$C_{\varepsilon_t} = C_\infty R\left(\frac{3}{2} + \delta, \eta\right) \left\{ \left(\frac{5}{2} + \delta\right) R\left(\frac{5}{2} + \delta, \eta\right) - \left(\frac{3}{2} + \delta\right) R\left(\frac{3}{2} + \delta, \eta\right) \right\}, \quad (3.55)$$

with $C_\infty = \left(\frac{3}{2} + \delta\right) Nk$.

3.5.2 Forced evaporative cooling

In forced evaporative cooling the escape threshold (ε_t) is lowered with decreasing temperature, thus allowing the evaporation to proceed at a desired rate. An approximately constant evaporation rate is obtained by keeping the truncation parameter (η) constant. Therefore, rather than describing the evaporation with Equation (3.53), in the case of forced evaporative cooling it is more convenient to use η rather than ε_t as the third independent thermodynamic variable and to write changes of the internal energy by

$$dE = C_\eta dT + \mu_\eta dN + W_\eta d\eta, \quad (3.56)$$

where $C_\eta = (\partial E / \partial T)_{N, \eta}$ is the heat capacity at constant truncation parameter $\mu_\eta = (\partial E / \partial N)_{T, \eta}$ is like a ‘chemical potential’ of evaporation at constant truncation parameter and $W_\eta = (\partial E / \partial \eta)_{N, T}$ is a heat of truncation at constant quasi-temperature and for a fixed number of atoms. With Equation (3.18) it follows immediately that

$$C_\eta = \left(\frac{3}{2} + \tilde{\gamma} + T (\partial \tilde{\gamma} / \partial T)_\eta\right) Nk \quad \text{and} \quad \mu_\eta = \left(\frac{3}{2} + \tilde{\gamma}\right) kT. \quad (3.57)$$

Note that $\mu_\eta = \mu_{\varepsilon_t} = E/N$ for the non-interacting Bose gas considered here.

For the special case of forced evaporative cooling at constant η the third term in Equation (3.56) does not contribute to the internal energy change, leaving only two independent thermodynamic variables, N and T . In this special case the expressions for forced evaporative cooling coincide with those of plain evaporative cooling provided C_{ε_t} is replaced by C_η .

Power-law traps: It follows with expression (3.20) for the $\tilde{\gamma}$ parameter that the chemical potential of evaporation and the heat capacity at constant truncation parameter are given by

$$C_\eta / Nk = \left(\frac{3}{2} + \delta\right) R\left(\frac{3}{2} + \delta, \eta\right). \quad (3.58)$$

3.5.3 The scaling parameters $\tilde{\alpha}$ and $\tilde{\beta}$

From section 3.4.4 we know the rate at which internal energy is removed from the sample by the escape of atoms. For quasi-static truncation of the distribution function the change of the internal may be expressed in terms thermodynamic variables of choice, N , T and ε_t or N , T and η . Here two *special cases* will be discussed: (a) plain evaporative cooling and (b) forced evaporative cooling *at constant* η . In both cases the thermodynamic properties depend only on two independent variables, N and T , and the rate of change of internal energy may be expressed in the same form,

$$\dot{E} = C_i \dot{T} + E \dot{N} / N, \quad (3.59)$$

where the subscript of C_i is used to indicate plain or forced conditions, with $i \in (\varepsilon_t, \eta)$ in accordance with eqs. (3.54) and (3.57), respectively. Equating Equation (3.59) with Equation (3.38) and using the property that for evaporation at constant η the quantity $\dot{\varepsilon}_t/\varepsilon_t$ may be replaced by \dot{T}/T we find

$$\tilde{\alpha} = \frac{d \ln T}{d \ln N} = \frac{\eta + (1 - X_{ev}/V_{ev}) - (\frac{3}{2} + \tilde{\gamma})}{C_i/Nk + (1 - X_{ev}/V_{ev})\tilde{\xi}_i}, \quad (3.60)$$

where the second terms in the denominator is only present in the case of forced cooling as is expressed by the Kronecker delta in the definition, $\tilde{\xi}_i \equiv \delta_{i,\eta}\tilde{\xi}$, of the parameter $\tilde{\xi}_i$. Here $\tilde{\xi}$ is the spilling parameter introduced in section 3.4.3. The scaling parameter $\tilde{\alpha}$ is an important quantity, expressing the efficiency of the cooling process. If $\tilde{\alpha}$ is negative the evaporation gives rise to heating. For $\tilde{\alpha} > 0$ this scaling parameter tells us how the quasi-temperature drops with atom loss during the evaporation process.

A related quantity, the scaling parameter $\tilde{\beta}$, tells us how the quasi-density scales with the quasi-temperature

$$\tilde{\beta} = \frac{d \ln n_0}{d \ln T}. \quad (3.61)$$

Using the identity $\dot{n}_0/n_0 = \dot{N}/N - \dot{V}_e/V_e$ and the scaling behaviour of the reference volume V_e with quasi-temperature and escape energy, given by $\dot{V}_e/V_e = \tilde{\gamma}\dot{T}/T + \tilde{\xi}\dot{\varepsilon}_t/\varepsilon_t$, we find (noting that for forced evaporative cooling at constant η the quantity $\dot{\varepsilon}_t/\varepsilon_t$ may be replaced by \dot{T}/T) the following expression for $\tilde{\beta}$

$$\tilde{\beta} = \frac{1}{\tilde{\alpha}} - (\tilde{\gamma} + \tilde{\xi}_i) \quad (3.62)$$

To have cooling with increasing n_0 the scaling parameter $\tilde{\beta}$ should be negative, corresponding to the condition $\tilde{\alpha} > 1/(\tilde{\gamma} + \tilde{\xi}_i)$ or, equivalently, the (recursive) condition

$$\eta > (\frac{3}{2} + \tilde{\gamma}) + \frac{C_i/Nk + \delta_{i,\eta}(1 - X_{ev}/V_{ev})\tilde{\xi}_i}{\tilde{\gamma} + \tilde{\xi}_i} - (1 - X_{ev}/V_{ev}) \quad (3.63)$$

The lowest η value at which this condition is satisfied will be called η_0 .

3.5.4 Run-away evaporation

Even with the truncation parameter constant and equal to η_0 (i.e., for constant n_0) the forced evaporation rate at constant η will slow down with falling temperature due to the thermal speed dependence of the atomic collision frequency $n_0\bar{v}\sigma$. In order to prevent this, the density n_0 should increase at least inversely proportional to $T^{1/2}$. This process in which the cooling rate speeds up is known as run-away evaporation. Using the identity $d(\ln n_0 T^{1/2})/dt = \dot{n}_0/n_0 + \frac{1}{2}\dot{T}/T$, the condition for run-away evaporation is seen to be given by the expression

$$\frac{d \ln n_0 T^{1/2}}{d \ln T} = \frac{1}{\tilde{\alpha}} - (\tilde{\gamma} + \tilde{\xi}) + \frac{1}{2} < 0, \quad (3.64)$$

i.e., $\tilde{\alpha} > 1/(\tilde{\gamma} + \tilde{\xi} - \frac{1}{2})$, so that for this case the recursive condition (3.63) should be replaced by the condition

$$\eta > \left(\frac{3}{2} + \tilde{\gamma}\right) + \frac{C_\eta/Nk + (1 - X_{ev}/V_{ev})\tilde{\xi}}{\tilde{\gamma} + \tilde{\xi} - \frac{1}{2}} - (1 - X_{ev}/V_{ev}). \quad (3.65)$$

The lowest η value at which this condition is satisfied will be called the critical truncation parameter η_c .

Examples

Plain evaporative cooling: To have cooling at initially constant n_0 , the parameter $\tilde{\beta}$ for the scaling of n_0 with temperature should be equal to zero at the start of the cooling process, i.e., the truncation parameter η should be equal to η_0 . Substituting the expressions (3.20), (3.55) and (3.41) for $\tilde{\gamma}$, C_{ε_t} and X_{ev}/V_{ev} , respectively, into Equation (3.63), and using Equation (3.28) for V_{ev}/V_e , we can solve for η_0 .

We first discuss the case of a 3D harmonic trap ($\delta = \frac{3}{2}$). Here we calculate $\eta_0 = 2.9$. With this value for η_0 we can inspect values for the thermodynamic quantities: $E/NkT = 1.8$, $C_{\varepsilon_t}/Nk = 0.44$ and calculate the ratios $X_{ev}/V_{ev} = 0.6$ and $V_{ev}/V_e = 0.5$. Then we can calculate the scaling parameters $\tilde{\gamma} = 0.29$ with Equation (3.20) and $\tilde{\alpha} = 3.4$ with Equation (3.60) to verify that indeed the scaling parameter $\tilde{\beta}$ is zero (i.e., $\tilde{\alpha} = 1/\tilde{\gamma}$). Then, the (initial) characteristic cooling time can be calculated with the following expression

$$-\frac{\dot{T}}{T} = \frac{1}{\tilde{\gamma}} n_0 \bar{v} \sigma e^{-\eta_c} V_{ev}/V_e \approx 0.1 n_0 \bar{v} \sigma. \quad (3.66)$$

Initially n_0 remains constant as the quasi-temperature drops. However, since ε_t is constant this leads to an increase in truncation parameter and n_0 will start to increase while the cooling rate is cut-off exponentially.

For several power-law traps, characterised by their δ value, the results for plain evaporation (constant ε_t) are summarised below:

δ	3	2.5	2	1.5	1	0.5
η_0	2.25	2.39	2.59	2.91	3.50	5.05
$\tilde{\alpha}$	5.0	4.5	3.9	3.4	3.0	3.0

For plain evaporation the spherical quadrupole traps ($\delta = 3$) are clearly favourable. Even for a truncation parameter as low as 2.25 the density grows monotonously for these traps. Also the large efficiency parameter $\tilde{\alpha}$, indicating that the temperature falls with the fifth power of the number of atoms remaining in the trap, is spectacular. This means that the spherical quadrupole trap is best suited to load a trap to the onset of evaporative cooling.

Forced evaporative cooling at constant η : Turning to forced evaporative cooling we consider two cases: (a) forced evaporative cooling at constant n_0 (i.e., $\eta = \eta_0$) and

(b) forced evaporative cooling at the onset of run-away evaporation (i.e., $\eta = \eta_c$). In both cases we consider power-law traps, so we may use the simplifying relation $\tilde{\gamma} + \tilde{\xi} = \delta$ (see section 3.4.3). The efficiency parameter ($\tilde{\alpha}$) may then be expressed as

$$\tilde{\alpha} = \frac{1}{\delta + \tilde{\beta}}, \quad (3.67)$$

where $\tilde{\beta}$ has the value 0, for forced evaporative cooling at constant n_0 , or $-\frac{1}{2}$, at the onset of run-away evaporation.

(a) For forced evaporative cooling at constant n_0 the evaporation process starts, as in the case of plain evaporation, with $\eta = \eta_0$. Lowering ε_t proportional to T , thus keeping η constant, causes the density n_0 to remain constant as can be seen from Equation (3.63) where T does not appear explicitly. The difference from plain evaporative cooling shows up in the value for the efficiency parameter ($\tilde{\alpha}$) which is readily calculated with Equation (3.67) by setting $\tilde{\beta}$ equal to zero.

δ	3	2.5	2	1.5	1	0.5
η_0	2.25	2.39	2.59	2.91	3.50	5.05
$\tilde{\alpha}$	1/3	2/5	1/2	2/3	1	2

Not surprisingly, the particle loss due to the ramp-down procedure is most pronounced for traps with the largest density of states near the truncation edge. This shows up in the efficiency parameter, $\tilde{\alpha}$. Similar behaviour can be found for the spilling parameter, $\tilde{\xi}$.

(b) Choosing η constant and equal to η_c the cooling not only *starts* at constant $n_0\bar{v}$ but also *continues* at constant $n_0\bar{v}$. This is the onset condition for run-away evaporation. As in the previous example the expression (3.67) holds, but now, in accordance with Equation (3.64), we require that the scaling parameter $\tilde{\beta}$ is less than $-\frac{1}{2}$. For 3D harmonic traps it follows with Equation (3.65) that $\eta_c = 4.59$ and $E/NkT = C_\eta/Nk = 2.41$. The volume ratios are given by $X_{ev}/V_{ev} = 0.42$ and $V_{ev}/V_e = 1.37$. For the scaling parameters we calculate $\tilde{\gamma} = 0.912$, $\tilde{\xi} = 0.588$ and $\tilde{\alpha} = 1$. The cooling rate may be expressed as

$$-\frac{\dot{T}}{T} = \frac{1}{\tilde{\gamma} - \frac{1}{2}} n_0 \sigma \bar{v} e^{-\eta_c} V_{ev}/V_e \approx 0.034 n_0 \sigma \bar{v}, \quad (3.68)$$

which is a factor 3 slower than the initial cooling rate given in expression (3.66) but has the advantage that the exponential throttling with falling quasi-temperature has been eliminated. Note that $\tau_t^{-1} = 1.4 \tau_{ev}^{-1}$. This means that we are at the edge of the quasi-static ramping regime and that more than half of the atoms are lost by spilling.

Comparing the various power-law traps for evaporation forced at run-away conditions we find the results compiled in the table below

δ	3	2.5	2	1.5	1	0.5
η_c	3.17	3.43	3.84	4.59	6.59	∞
$\tilde{\alpha}$	2/5	1/2	2/3	1	2	-

Both examples of forced evaporative cooling show that high- δ traps require the smallest truncation parameter to move at the desired slope through the $n_0 - T$ phase diagram. This is a nice feature because it enables fast cooling. However, by comparing the $\tilde{\alpha}$ parameters we see that the low- δ traps are more efficient. This raises the question how the various traps compare (under forced evaporative cooling at constant η) for equal values of the truncation parameter. This comparison was made for $\eta = 4.59$, the critical truncation value for run-away evaporation in harmonic traps. The results are presented below

δ	3	2.5	2	1.5	1	0.5
$\tilde{\alpha}$	0.54	0.64	0.79	1	1.31	1.8

Note that also at equal η the harmonic traps are more efficient than spherical quadrupole traps. However, since in this case the high- δ traps are operated well inside ‘the run-away regime’ ($\eta \approx 1.5 \eta_c$) the evaporation speeds up (due to a strong increase in n_0 and related to the strong T dependence of the effective volume). This run-away may be an important advantage in cases where short cooling times are required.

Appendix: Incomplete gamma functions

The incomplete gamma function is defined by

$$P(a, \eta) \equiv \frac{1}{\Gamma(a)} \int_0^\eta dt t^{a-1} e^{-t}, \quad (3.69)$$

where $\Gamma(a)$ is the Euler gamma function. $P(a, \eta)$ grows monotonically from zero to one for increasing $\eta \geq 0$. $P(a, \eta)$ can be expressed as a series expansion

$$P(a, \eta) = e^{-\eta} \eta^a \sum_{m=0}^{\infty} \frac{\eta^m}{\Gamma(m+a+1)} \quad (3.70)$$

which reduces for integer $a = 1, 2, 3, \dots$ to

$$P(a, \eta) = 1 - e^{-\eta} \sum_{m=0}^{a-1} \frac{\eta^m}{m!}. \quad (3.71)$$

Expansion in terms of $1/\eta$:

$$P(a, \eta) = 1 - e^{-\eta} \frac{\eta^{a-1}}{\Gamma(a)} \left[1 + \frac{(a-1)}{\eta} + \frac{(a-1)(a-2)}{\eta^2} + \dots \right] \quad (3.72)$$

The derivative of $P(a, \eta)$ with respect to η is given by

$$\frac{\partial P(a, \eta)}{\partial \eta} = \frac{a}{\eta} [P(a, \eta) - P(a+1, \eta)] = \frac{e^{-\eta} \eta^{a-1}}{\Gamma(a)} \quad (3.73)$$

and, hence

$$R(a, \eta) \equiv \frac{P(a+1, \eta)}{P(a, \eta)} = 1 - e^{-\eta} \frac{\eta^a}{\Gamma(a+1)} \frac{1}{P(a, \eta)}. \quad (3.74)$$

A useful recursion relation for $R(a, \eta)$ functions is

$$\frac{1}{R(a, \eta)} = 1 + \frac{a+1}{\eta} [1 - R(a+1, \eta)]. \quad (3.75)$$

The derivative of $R(a, \eta)$ with respect to η is given by

$$\frac{\partial R(a, \eta)}{\partial \eta} = \frac{R(a, \eta)}{\eta} [1 + aR(a, \eta) - (a+1)R(a+1, \eta)]. \quad (3.76)$$

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