Non-Equilibrium Quantum Statistics of Trapped Ideal Bose Gases

Diploma Thesis
by
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Submitted to the
Department of Physics
Freie Universität Berlin
August 14, 2009

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To my parents,
who supported me along the way.

Chapter 1

Introduction

In the following, we give a brief historical introduction to the subject of ideal quantum gases and to the phenomenon of Bose-Einstein condensation, which takes place in these systems for low enough temperatures and in equilibrium conditions. We outline the mathematical description in terms of critical parameters, before we continue with non-equilibrium phenomena, where we present two important examples related to quenches of a parameter of the underlying Hamiltonian.

1.1 Ideal Quantum Gases in Equilibrium

In 1920, the Indian physicist Satyendra Nath Bose wrote a paper on the quantum statistics of light quanta (photons), in which he argued that Maxwell-Boltzmann statistics might not be the right statistics for microscopic particles, where fluctuations due to the uncertainty principle will be significant. In his derivation of the right statistics for a photon gas he assumed that the number of quantum states available to a single photon of fixed energy is given by the number of phase space cells of volume h^3, using only Einstein's light quantum hypothesis and the laws of statistical physics and obtaining a version of Planck's law at the end.

However, European physics journals refused to publish his results, as it was their contention that Bose was mistaken. Discouraged, he sent his work to Albert Einstein in 1924, who immediately recognised its significance and arranged its publication in the *Zeitschrift für Physik* after he had translated it to German [1].

Einstein extended Bose's work to an ideal gas of massive particles, publishing his results in a first article [2] some months later. In a follow-up article [3], he noted that from the equation of state of this ideal quantum gas there follows a critical particle density, where further compression results in the *condensation* of additional particles into the lowest quantum state, i.e. the ground state.

From a modern perspective, the principle behind what is today known as Bose-Einstein condensation can be understood by the following argument: Consider a collection of N non-interacting particles which can each be in one of two quantum states $|0\rangle$ and $|1\rangle$, both having *equal energy*.

If the particles are assumed to be distinguishable, there are 2^N possible configurations, i.e. microstates of this system. Let p_1 and $p_2 = 1 - p_1$ be the a priori probability for a particle to be in $|0\rangle$ and $|1\rangle$, respectively, then the probability that k particles are in state $|0\rangle$ and $N-k$ in state $|1\rangle$ is given by the probability function of the binomial distribution

$$\rho_{\mathrm{D}}(k, N) = p_1^k (1-p_1)^{N-k} \binom{N}{k} . \tag{1.1}$$

If each particle may be in $|0\rangle$ or $|1\rangle$ independently and with equal probability, i.e. $p_1 = p_2 = 1/2$, which is the *equal a priori probability postulate* of statistical mechanics, we have specifically

$$\rho_{\mathrm{D}}(k, N) = \left(\frac{1}{2}\right)^k \left(1 - \frac{1}{2}\right)^{N-k} \binom{N}{k} = \frac{1}{2^N}\binom{N}{k} \, . \tag{1.2}$$

This expression has a maximum for $k = N/2$, i.e. when both states are equally populated. It follows that in almost all the possible configurations of the system, about half of the particles will be in $|0\rangle$ and the other half in $|1\rangle$. Thus, this balance is a statistical effect; the number of configurations is largest when the particles are divided equally.

If the particles are indistinguishable, however, there are only $N + 1$ different configurations, since it cannot be determined if a certain particle is in $|0\rangle$ or $|1\rangle$. Consequently, each value of k determines a unique quantum state for the whole system. If these states all have the same probability, there is no statistical spreading out; i.e. it is equally likely for all the particles to sit in $|0\rangle$ as to be equally partitioned between both states.

Suppose now that the energy of state $|1\rangle$ is slightly larger than the energy of state $|0\rangle$ by an amount E. At temperature T, a particle will have a lesser probability to be in state $|1\rangle$ by a Boltzmann weight $\exp\{-E/T\}$. In the distinguishable case, the particle distribution will be biased slightly towards state $|0\rangle$ and the distribution will be slightly different from half and half. But in the indistinguishable case, since there is no statistical pressure toward equal occupation numbers, the most likely outcome is that most of the particles will collapse into state $|0\rangle$:

In the indistinguishable case, each value of k has its separate Boltzmann probability of $\exp(-\beta E k)$, so the probability distribution is exponential. Introducing for convenience $k' = N - k$ for the number of particles in state $|1\rangle$, we have

$$\rho_{\mathrm{I}}(k', N) = C\,\mathrm{e}^{-\beta E k'} = C\,p^{k'} \, , \tag{1.3}$$

where C is a normalisation constant. In the thermdynamic limit $N \to \infty$, the sum $\sum_{k'=0}^{\infty} p^{k'}$ yields $C = 1-p$ and the number of particles that are not in state $|0\rangle$ is given by the expectation value of the particle number n:

$$\langle n(k)\rangle = C\sum_{n>0}^{\infty} n\,p^n = \frac{p}{1-p} = \frac{1}{\mathrm{e}^{\beta E} - 1} \, , \tag{1.4}$$

which is a constant as $N \longrightarrow \infty$. It follows that for a collection of a large number of bosons (i.e. particles with integer spin) in equilibrium, at low temperatures most will be in the ground state $|0\rangle$ of the system and only a negligible amount in thermally excited states. Thus at its heart, Bose-Einstein condensation is a quantum statistical effect, as it can only take place in ensembles of indistinguishable particles.

Mathematically, this can be seen as follows. For an ideal quantum gas of bosons in thermodynamic equilibrium, the mean occupation number of the single-particle state i in the grand-canonical description is given, according to Einstein, by what today we know as the Bose-Einstein distribution function:

$$n(E_i) = \frac{1}{\mathrm{e}^{\beta(E_i - \mu)} - 1} \, . \tag{1.5}$$

Here, $\beta = 1/k_\mathrm{B}T$ is the inverse temperature, k_B is the Boltzmann constant and μ is the chemical potential, which is determined implicitly by the condition that the sum of all occupation numbers (1.5) must yield the total particle number N, i.e.

$$N = \sum_i \frac{1}{\mathrm{e}^{\beta(E_i-\mu)} - 1} \,. \tag{1.6}$$

Dividing (1.6) by the volume V that the system occupies, gives the particle density $n(E_i)$ which we have sloppily denoted by the same symbol as the occupation number. In the thermodynamic limit of an infinite system $N \to \infty$ and $V \to \infty$, such that the density $n = N/V$ remains constant, the sum in (1.6) becomes an integral with the substitution $1/V \to 1/(2\pi\hbar)^3$ and we have

$$n(\mathbf{p}) = \frac{1}{(2\pi\hbar)^3} \int d^3p \, \frac{1}{\mathrm{e}^{\beta(\mathbf{p}^2/2M-\mu)} - 1} \,. \tag{1.7}$$

This is a monotonously increasing function of μ, which is bounded as $\mu \nearrow 0$ by the critical density

$$n_\mathrm{c} = \left(\frac{Mk_\mathrm{B}T}{2\pi\hbar^2}\right)^{3/2} \zeta(3/2) \,, \tag{1.8}$$

where $\zeta(3/2) \approx 2.612$. This is absurd, of course and the resolution is that the particles exceeding the critical number all go into the lowest energy state. Thus, below the corresponding critical temperature

$$T_\mathrm{c} = \frac{2\pi\hbar^2}{Mk_\mathrm{B}} \left[\frac{n_\mathrm{c}}{\zeta(3/2)}\right]^{2/3} \,, \tag{1.9}$$

the ground state of the gas is macroscopically populated and accordingly one has to be more careful in replacing the sum in (1.6) by an integral. To this end, it is sufficient to separate the contribution from the ground state, i.e. the condensate fraction, and to approximate the thermal contribution by an integral:

$$n = n_0 + n(\mathbf{p}) \,. \tag{1.10}$$

According to the wave-particle duality, the particles in the Bose gas must be taken to be wave packets. Their mean temperature dependent wavelength is then of the order of the so-called thermal de Broglie wavelength

$$\lambda_\mathrm{dB} = \left(\frac{2\pi\hbar^2}{Mk_\mathrm{B}T}\right)^{1/2} \,. \tag{1.11}$$

Now, using (1.11) and noting, that the mean interparticle spacing is of order of the third root of the inverse particle density, $n^{-1/3}$, equation (1.9) reads

$$n_\mathrm{c}\,\lambda_\mathrm{dB}^3 = \left(\frac{\lambda_\mathrm{dB}}{n^{-1/3}}\right)^3 = \zeta(3/2) \,. \tag{1.12}$$

Thus, we see that Bose-Einstein condensation sets in, when the mean interparticle spacing becomes comparable to the particle's thermal de Broglie wavelength. As the wavefunctions of the particles start to overlap, they begin to take up the same region of space, so quantum statistics, i.e. the symmetry of the many-particle wavefunction becomes important and we are now dealing with a true quantum gas.

Apparently, there are two ways that this condition can be met: First, by lowering the temperature and thus increasing the thermal de Broglie wavelength (1.11); and secondly, by increasing the particle density and therefore decreasing the mean interparticle spacing. However, at low enough temperatures, the particles of all substances have the natural tendency to clog together and eventually solidify. This solidification process typically proceeds via two mechanisms: By three-body and higher order inelastic collisions of the particles; and by collisions of the gas particles with the walls of their container. The second problem may be avoided by keeping the gas sample strictly isolated from the walls of its container; this is done by trapping it in ultra high vacuum (UHV) conditions inside a variety of magnetic fields, the potentials of which are in most cases well approximated by that of an anisotropic harmonic oscillator.

Since the probability of three-body collisions is proportional to the cube of the particle density, n^3, it follows that in order to achieve Bose-Einstein condensation, n must be low enough, so that three-particle collisions are negligible, and consequently BEC is only achievable in very dilute gases of typically 10^{13}–10^{15} atoms/cm^3, requiring extremely low temperatures of the order of microkelvins [15]. On the other hand, since BEC is a phase transition that requires thermal equilibrium, two-body collisions, the rate of which is proportional to n^2, must be sufficiently frequent to allow the particles to equilibrate. The regime in the phase diagram where BEC takes place is thus metastable and the condensates are lost after a time of a few seconds to several minutes, when the system eventually goes into the thermodynamically stable solid phase.

The lack of suitable cooling and trapping techniques is the main reason for the relatively late experimental realisation of BEC in the mid 1990s. Early experiments with dilute gases in the 1980s had mainly focused on spin-polarised hydrogen and it was for this system, that evaporative cooling was invented in 1985. With evaporative cooling, the magnetic trapping potential is lowered, so that the most energetic particles can escape; thus the high energy tail of the thermal distribution is constantly removed from the trap. Of course, in order for this process to take place continuously, the thermal tail must constantly be repopulated and this requires short thermalisation times, which in turn requires high particle densities.

A major step forward to the demonstration of BEC was the combination of laser cooling and evaporative cooling in 1994, which extended the applicability of evaporative cooling to alkali atoms, as well as the introduction of radio frequency induced evaporative cooling, which made the technique more efficient.

Laser cooling is an application of the Doppler effect, where two counterpropagating laser beams of equal intensity and frequency are focused on the gas cloud. If the frequency of the laser beams is slightly detuned from the frequency of an optical transition from the ground state to an excited state of the atomic species to be cooled, an atom which is at rest absorbs equally many left-moving photons as right moving ones, each of which imparts momentum of $p = \hbar\mathbf{k}$ on the atom, so the total momentum change will be zero. However, an atom which moves to the right will absorb less right-moving photons, as their frequency is Doppler-shifted away from the transition, and more left-moving photons, as it "sees" their Doppler-shifted frequencies closer to the transition frequency. Thus the laser fields produce a "frictional", i.e. velocity dependent force on the atoms, so the cloud is effectively cooled.

The first Bose-Einstein condensate was then observed in 1995 by Eric Cornell and Carl Wieman at the University of Colorado using a gas of approximately 2×10^4 rubidium atoms cooled to 170 nK [4]; and shortly afterwards in a sample of 10^5 lithium atoms [6], as well as in 5×10^5 sodium atoms by the group of Wolfgang Ketterle at MIT [7]. This discovery was honoured with the 2001 Nobel Price in Physics for Cornell, Wieman, and Ketterle.

The unique feature of a BEC lies in the fact, that it is a macroscopic quantum object, where the individual bosons are completely delocalised. A BEC consists of a single macrosopic wavefunction, which displays all the features of quantum mechanics – such as quantum coherence – on macroscopical length scales.

1.2 Non-Equilibrium Phenomena

Despite the fact that the study of the equilibrium properties of systems is one of the most important tools in statistical physics, it is important to note that generally all systems are constantly in a non-equilibrium state; although they may be very close to equilibrium on some timescale. Real systems are not isolated from their environment and are therefore continuously interacting and interchanging energy with other systems. This sharing of energy includes being driven by external energy sources as well as dissipating energy to the environment.

Thus experimentally, the notion of equilibrium state is an approximation. It is limited by power on and power off cycles of the experimental apparatus, by imperfect isolation of the system being studied from the environment of the containing vessel, as well as by changes in different parameters as the experiment progresses.

Mathematically, the main point in the description of non-equilibrium phenomena is that the system in question is governed by a time dependent Hamiltonian $\hat{H}(t)$ that does not commute for different times, i.e. $[\hat{H}(t_1), \hat{H}(t_2)] \neq 0$. There exist different classes of methods for the theoretical description of time dependent quantum systems.

If the system is subject to small time dependent perturbations, the Hamiltonian may be split into a time independent and a time dependent part via

$$\hat{H}(t_1) = \hat{H}_0 + \lambda \, \hat{H}_1(t) \; , \tag{1.13}$$

with λ being a small quantity associated with the size of the perturbation. This approach leads to time dependent perturbation theory, where in the end one obtains an expression for the physical quantity of interest (e.g. time dependent expectation values, time dependent amplitudes of energy eigenstates of the unperturbed system) as an infinite power series in λ.

Instead of (1.13) the time dependence of the system may be such, that a system parameter is changed on a short timescale. In many cases these changes are so fast, that one may consider the limit of a sudden, abrupt change. The system is prepared, for instance, in the ground state of an *initial* Hamiltonian $\hat{H}_{\mathrm{I}}$. At time t_0 the system parameter is then changed instantly, in the following of which the system evolves under the influence of a *final* Hamiltonian $\hat{H}_{\mathrm{F}}$. This situation is called a quench. Such a quench is an example of a particularly simple non-equilibrium situation, since for its description only two non-commuting Hamiltonians are required, instead of the infinitely many in the general case (1.13). In the following, we give two important examples of non-equilibrium phenomena in the field of Bose-Einstein condensation, both of which can be regarded as quenches. The first is the turning-off of all trapping potentials prior to the recording of so-called time-of-flight images. The second is the observation of collapse and revival of the condensate field in an optical lattice following a quench of the lattice potential.

1.2.1 Time-of-Flight Imaging

Different methods exist for the detection and observation of a Bose-Einstein condensate. One of the oldest methods is time-of-flight imaging, where the trapping potentials are suddenly turned off and the density of the expanding atomic cloud is imaged. We note, that this turning-off of all trapping potentials can be regarded as a special quench in the trap frequency, where ω is taken from its normal value to zero.

For a harmonic trap and for times much larger than the inverse of the associated oscillator frequency, i.e. for $\omega t \gg 1$, the recorded density profiles for the thermal and the condensate component are proportional to their respective momentum distributions, as we will see below. The thermal component of an harmonically trapped quantum gas in three dimensions may be described semiclassicaly by its density function

$$n_{\mathrm{T}}(\mathbf{r}) = \lambda_{\mathrm{dB}}^{-3}\, \zeta_{3/2}\left(\mathrm{e}^{\beta(\mu - V(\mathbf{r}))}\right) , \tag{1.14}$$

where

$$V(\mathbf{r}) = \sum_{i=1}^{3} \frac{M}{2} \omega_i^2\, x_i^2 \tag{1.15}$$

is the harmonic potential. When the trap is switched off, the atoms fly ballistically from their position in the trap with the velocity at the time of the switch-off. For an atom that starts at point $\mathbf{r}_0$ and arrives at $\mathbf{r}$ after a time t of free expansion, the momentum is $\mathbf{p} = M(\mathbf{r} - \mathbf{r}_0)/t$. After an expansion time of t, the distribution is the given by

$$n_{\mathrm{T}}(\mathbf{r}, t) = n_{\mathrm{T}}(\mathbf{r} - \mathbf{p}t/M) . \tag{1.16}$$

Using (1.5), we may determine the density distribution as a function of the expansion time t by performing an integration over momentum, i.e. $n_{\mathrm{T}}(\mathbf{r}, t) = (M/t)^3 \int d\mathbf{p}\, n_{\mathrm{T}}(\mathbf{r} - \mathbf{p}t/M)$, yielding

$$n_{\mathrm{T}}(\mathbf{r}, t) = \lambda_{\mathrm{dB}}^{-3} \left[\prod_{i=1}^{3} \left(\frac{1}{1 + \omega_i^2 t^2}\right)^{1/2}\right] \zeta_{3/2}\Big(\exp\left\{\beta\left[\mu - \sum_i \frac{M\omega_i^2 r_i^2}{2(1 + \omega_i^2 t^2)}\right]\right\}\Big) . \tag{1.17}$$

As it was said above, for large times, i.e. $t \gg \omega_i^{-1}$, the density distribution of the thermal cloud becomes isotropic:

$$n_{\mathrm{T}}(\mathbf{r}, t) \xrightarrow{t \gg \omega_i^{-1}} \lambda_{\mathrm{dB}}^{-3}\, \zeta_{3/2}\left(\mathrm{e}^{\beta(\mu - \frac{Mr^2}{2t^2})}\right) . \tag{1.18}$$

For noninteracting particles, the ground state wavefunction is a Gaussian, and consequently the condensate density is also a Gaussian, given by

$$n_0(\mathbf{r}) = N_0 \pi^{-3/2} \prod_{i=1}^{3} r_{i,0}^{-1} \exp\left\{-\left(\frac{r_i}{r_{0,i}}\right)^2\right\} . \tag{1.19}$$

Under unitary time evolution, Gaussian wavepackets remain Gaussian except for a phase factor. Thus, after a time t of free expansion, the oscillator length $r_{0,i} = \sqrt{\hbar/M\omega_i}$ in (1.19) is simply rescaled [5] according to

$$r_{i,0}'^2 = r_{0,i}^2 + v_i^2 t^2 = \frac{r_{0,i}^2}{1 + \omega_i^2 t^2} , \tag{1.20}$$

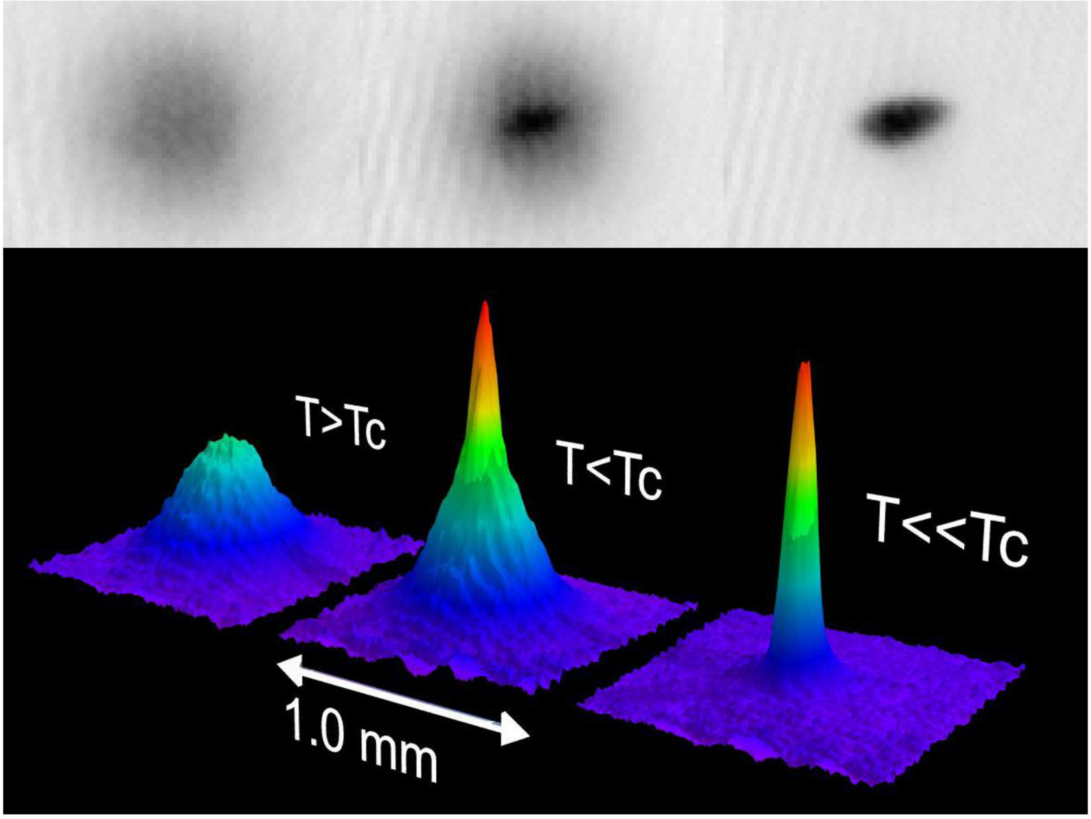

Figure 1.1: Observation of Bose-Einstein condensation of sodium atoms by absorption imaging. Each of the three images was taken after a time-of-flight of 6 ms. They show, from left to right, an expanding cloud cooled to: just above the critical temperature $T > T_\mathrm{c}$, just below, after the condensate appeared, and well below T_c, showing an almost pure condensate . Images taken in 1995 by the group of Wolfgang Ketterle and Dave Pritchard at MIT [7].

where $v_i = \sqrt{\hbar\omega_i/M}$ is the velocity associated with harmonic oscillator's ground state energy. Therefore, we obtain the following expression for the time dependent density of the expanding condensate:

$$n_0(\mathbf{r},t) = N_0 \prod_{i=1}^{3} \left(\frac{1}{1+\omega_i^2 t^2}\right)^{1/2} \sqrt{\frac{\pi\hbar}{M\omega_i}} \exp\left\{-\frac{M\omega_i r_i^2}{\hbar(1+\omega_i^2 t^2)}\right\} . \tag{1.21}$$

Among the different techniques that exist for visualising the velocity distribution of the trapped atoms, more precisely its density, there are absorption imaging and phase-contrast imaging [5]. In absorption imaging, light at a resonant frequency of the atomic species is passed through the atomic cloud and is partially absorbed. The absorption profile then yields information about the density distribution of the cloud. A drawback of absorption imaging is that it is destructive, since the absorption of light quanta heats the cloud considerably.

An alternative technique is phase-contrast imaging, which exploits the fact that the refractive index of the gas depends on its density. By allowing a light beam that has passed through the cloud to interfere with a reference beam that has been phase shifted, changes in optical path length are converted into intensity variations. This method is almost non-destructive.

After the light has passed through the thermal cloud and the condensate, both methods capture the resulting image via sensitive charge-coupled devices (CCD). The resulting time-of-flight images generally exhibit a narrow central peak which has the parabolic profile of the bottom of the trap, corresponding to the fraction of condensed bosons which have zero momentum, sitting collectively in the lowest eigenstate of the trapping potential, as well as a broad Gaussian distribution of the thermal component of the gas, which expands quickly. This sharp central peak in the velocity distribution of a harmonically trapped Bose gas is direct evidence for Bose-Einstein condensation.

Weakly interacting Bose gases are described by the Gross-Pitaevkii equation and in the limit of negligible kinetic energy and large particle numbers, we may apply the Thomas-Fermi approximation [16, Chapter 6.2], which yields for harmonic potentials $V(\mathbf{r})$ a density distribution of the form of an inverted parabola,

$$n_0(\mathbf{r}) = |\psi(\mathbf{r})|^2 = \left[\mu - V(\mathbf{r})\right]/U_0 \, , \tag{1.22}$$

where U_0 is associated with the interaction energy. Thus, as a result of the residual repulsive interaction, the density profile of the BEC deviates from a Gaussian and the expanding BEC retains the shape of the potential at the bottom of the trap. Consequently, it displays the same anisotropy in time-of-flight images, whereas the thermal cloud is spherically symmetric due to the isotropy of the velocity distribution (1.18). The observation, that the alleged condensate fraction retains the anisotropy of the trapping potential served as strong evidence for Bose-Einstein condensation in early experiments.

Figure 1.1 shows absorption images of the expanding cloud of an ultracold gas of sodium atoms, taken after the turning-off of the harmonic trapping potential, after a time-of-flight of 6 ms. The total number of atoms at the phase transition at $T_\mathrm{c} \approx 2\ \mu\mathrm{K}$ was approximately $N_\mathrm{tot} \approx 7 \times 10^5$. These images were recorded by the group of Wolfgang Ketterle and Dave Pritchard at MIT during their experiments in 1995, where the first BEC with sodium atoms was achieved [7].

The greyscale images in the top row are the original two dimensional absorption images; in the lower row, these were rendered in a three-dimensional plot where the blackness of the shadow is represented by height. The left image of Fig. 1.1 shows the expanding thermal cloud at just above the critical temperature T_c, where Bose-Einstein condensation sets in. Consequently, we only see the broad thermal distribution of an ultracold gas that still behaves classically. The image in the center was taken at a temperature just below T_c. Now, in the center of the thermal distribution, we see the sharp peak that accompanies the beginning of BEC. The density distribution is thus bimodal, with two separate contributions from the thermal component and the condensate. In the corresponding greyscale image above, we further observe that the BEC component displays the anisotropy discussed above. Finally, the third image was taken at a temperature well below the critical one, where most of the atoms are in the condensate component. Thus, the thermal component of the gas is practically absent and what is left is an almost pure Bose-Einstein condenstate.

1.2.2 Collapse and Revival in Optical Lattices

Bose-Einstein condensates may be loaded into two- or three-dimensional optical lattices; these are made by interfering counterpropagating laser beams such that at every location of the resulting grid of laser light where beams cross, a small potential well is formed, which can be used to trap neutral atoms via the Stark shift. The resulting periodic potential can then be populated by atoms from a condensate, so that the resulting system of trapped atoms resembles an ideal crystal [9, 10]. Today, these optical lattices are an important tool for condensed matter research, as they offer a toy model of a quantum solid-state system where all parameters, such as lattice spacing and depth of the periodic potential, can at least in principle be controlled. Thus, they allow researchers to simulate important aspects and phenomena of solid-state physics with a minimally complex system.

Optical lattices, that are populated with bosons, are described by the Bose-Hubbard model, the Hamiltonian of which reads

$$\hat{H}_{\mathrm{BH}} = -J \sum_{\langle i,j \rangle} \left(\hat{b}_i^\dagger \hat{b}_j + \hat{b}_j^\dagger \hat{b}_i \right) + \sum_i \left[\frac{U}{2} \hat{n}_i (\hat{n}_i - 1) - \mu_i \hat{n}_i \right] , \tag{1.23}$$

where the first part describes the hopping, or tunnelling, of particles between neighbouring sites with the hopping matrix element J, and the second is the on-site repulsion between particles in the same potential well, which is characterised by the on-site interaction matrix element U. Finally, $\hat{n}_i = \hat{b}_i^\dagger \hat{b}_i$ is the occupation number operator at site i and $\mu_i = \mu - M\omega^2 \mathbf{x}_i^2/2$ denotes the local chemical potential within the Thomas-Fermi approximation. This site dependence of μ_i is a consequence of the additional harmonic trapping potential which is usually superimposed on the optical lattice one.

In equilibrium, this model exhibits a quantum phase transition at a critical value of the interaction strength $U/J = u_{\mathrm{c}}$, between a superfluid ($U/J < u_{\mathrm{c}}$) and a Mott-insulating state ($U/J > u_{\mathrm{c}}$) [8]. For weak interactions relative to the kinetic energy, i.e. for $U/J \ll 1$, the system forms a Bose-Einstein condensed state of matter, where each atom is delocalised over the entire lattice. This state is favoured as the kinetic energy term in (1.23) is minimised for single-particle wavefunctions spread out throughout the lattice, so in this case the system is described by a single multiparticle wavefunction. This phase is referred to as the superfluid phase of the system. Superfluids (like the superfluid phase of helium) are extraordinary quantum liquids. They are generally characterised by a single coherent wavefunction, zero viscosity, as well zero entropy and infinite thermal conductivity.

In contrast, for the case of $U/J \gg 1$, i.e. when the on-site interactions are large compared to the kinetic energy, the system is in the Mott insulator phase, in which the atoms are localised at single lattice sites, with a fixed particle number per site. Therefore, the single site wavefunctions cannot overlap coherently, and the system cannot be described by a single coherent macroscopic wavefunction. Then, for very strong interactions, no interference pattern is observed [9, 10].

In an optical lattice, the potential well formed by the crossing laser beams at each lattice site can be prepared in a coherent superposition of different occupation number states with constant relative phases between neighbouring sites. These can be expressed as a superposition of eigenstates $|n\rangle$ of (1.23) at a single site with a complex amplitude α:

$$|\alpha\rangle = \mathrm{e}^{-i\frac{|\alpha|^2}{2}} \sum_n \frac{\alpha^n}{\sqrt{n!}} |n\rangle . \tag{1.24}$$

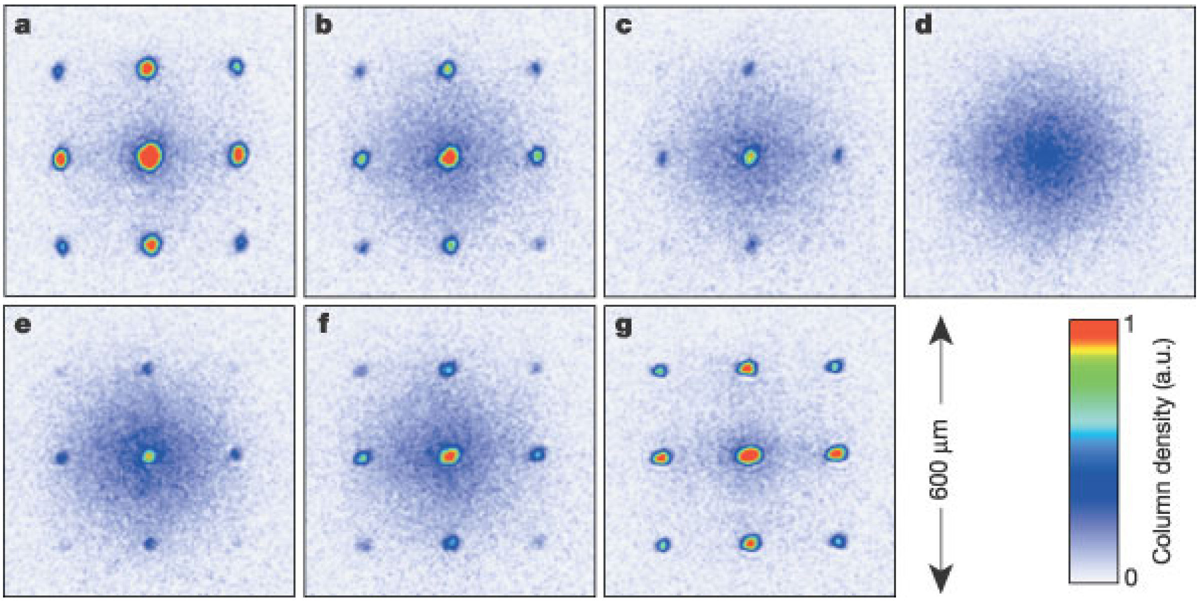

Figure 1.2: Absorption images of the dynamical evolution of the multiple matter wave interference pattern observed after quenching the optical lattice potential from the superfluid phase to the Mott insulator regime [11].

We obtain a time evolved coherent state (1.24) by using the solution of the Schrödinger equation for a Fock state, $|n\rangle(t) = |n\rangle(0)\,\exp\{-iE_n t/\hbar\}$:

$$|\alpha\rangle(t) = \mathrm{e}^{-i\frac{|\alpha|^2}{2}} \sum_n \frac{\alpha^n}{\sqrt{n!}} \mathrm{e}^{-iE_n t/\hbar} |n\rangle(0) \; . \tag{1.25}$$

In Ref. [11], Greiner et al. report on an experiment, where all lattice sites were initially prepared in such a superposition and where subsequently the lattice intensity was suddenly increased, taking the system from the superfluid phase to the Mott insulator regime. Following this quench, a periodic series of collapses and revivals of the collective interference pattern was observed. Figure 1.2 shows a series of seven experiments, where each time the intensity of the lattice potential was quenched. After each quench followed a variable hold time t, during which no further manipulations were performed on the system. After this hold time, all potentials were shut off and absorption images were taken. In the first image, **a**, of Fig. 1.2, the hold time was zero and consequently the quench could not affect the system. We see the typical momentum distribution of a square optical lattice, which can be thought of as a direct image of the reciprocal lattice. Thus, initially, the system can be described by a macroscopic wave function with *phase coherence* between individual potential wells.

In images **b** through **d**, taken after hold times of 100 μs , 150 μs, and 250 μs, the sharp interference peaks vanish completely, corresponding to a collapse of the macroscopic wavefunction over the entire lattice. Then, in images **e** through **f**, the interference pattern appears again, and is perfectly restored in image **g**, which was taken after 550 μs.

Thus, Figure 1.2 shows a complete cycle of collapse and revival of the multiple matter wave in an optical lattice. The strength of these oscillations, i.e. the number of coherent atoms relative

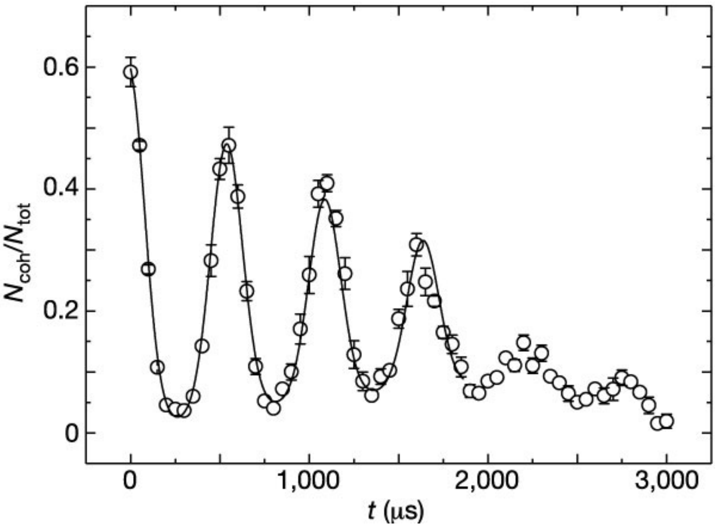

Figure 1.3: Number of coherent atoms relative to the total number of atoms monitored over time for the same experimental sequence as in Fig. 1.2. The solid line is a fit to the data assuming a sum of Gaussians with constant widths and constant time separations, including an exponential damping and a linear background, [11].

to the total number of atoms for the same experiments as above is depicted in Fig. 1.3. Here, the number of coherent atoms, N_{coh}, has relaxed to zero after 3 ms and about five complete cycles. The data points in Fig. 1.3 were fitted with a sum of Gaussians and an exponential damping term. According to the authors of [11], the damping is mainly an artefact of the measuring process: Due to the additional harmonic trap, that is superimposed on the optical lattice potential, the chemical potential in (1.23) is site-dependent and features a parabolic profile over the whole lattice, which leads to a broadening of the interference peaks over time. The density, however, is only counted inside a rectangular area of $130\,\mu\text{m} \times 130\,\mu\text{m}$ around the interference peaks of Fig. 1.2, so when these become broader than this area, N_{coh} cannot be correctly determined any more.

The apparent decay of oscillations in Fig. 1.3 can be modeled with the following approach due to Santos and Pelster [13]: Before the quench, the system is deep inside the superfluid phase and is thus well described by the Gross-Pitaevskii equation, where the collective wave function, or order parameter field $\psi_i(t) = \langle \hat{b}_i(t) \rangle$ is large.

Near the boundary to the Mott phase, however, ψ_i is small, so the system is better described by a Ginzburg-Landau theory, where the order parameter field ψ_i satisfies equations of motion that follow from an effective action [14]. In the limit of $U \to 0$ these equations of motion then reduce to the Gross-Pitaevskii equation. They may be linearised in ψ_i in order to treat small oscillations of the system, yielding the general solution in the time domain

$$\psi_i(t) = A_i^+ \mathrm{e}^{-i(Un_i - \mu_i)t/\hbar} + A_i^- \mathrm{e}^{-i[Un_i(n_i-1) - \mu_i]t/\hbar} \,. \tag{1.26}$$

Starting with the time-independent Gross-Pitaevskii equation, which is accurate only for the beginning of the quench, and at non-zero hopping, i.e. $J \neq 0$, the hopping constant is then quenched to $J = 0$ by changing the lattice potential. This causes the values of the parameters U and μ_i in (1.23) to change as well, i.e. to take on the values $\widetilde{U}$ and $\widetilde{\mu}_i$. The Gross-Pitaevskii equation in terms of these changed parameters has exact solutions for $J = 0$, which determine the boundary conditions for (1.26), i.e. the parameters $A_i^{\pm}$. From (1.26) one then obtains the momentum space distribution, from which the density at momentum $\mathbf{k}_\perp$ in the x-y-plane follows by integrating out the z coordinate. For large times $t \to \infty$ the integrated momentum space density turns out to have the asymptotical limit

$$n(\mathbf{k}_\perp, t) \propto \left(\frac{2\pi\hbar}{M\omega^2 a^2 t} \right)^2 , \tag{1.27}$$

with the lattice constant a. The condensate fraction in a small region δk^2 of $\mathbf{k}_\perp$-space around an interference peak is then of the form

$$N_\mathrm{c} \sim \frac{\alpha + \beta \cos\left(Ut/\hbar\right)}{t^2} , \tag{1.28}$$

where α and β are constants that can be explicitly determined in terms of the parameters $A_i^{\pm}$. Thus, it follows that the single-site order parameter field described by $\psi_i(t)$ has a periodic time dependence with a quadratic decay. This decay however, is no real damping due to dissipative processes, but a mere artifact of the experimental detection process.

1.3 Overview of this Thesis

This thesis is divided into two parts. The first consists of Chapters 2 and 3 and provides the necessary background for the statistical description of harmonically trapped ideal quantum gases. Therein, Chapter 2 deals with the description of many-particle systems: We start by introducing permutations and the corresponding symmetric group, as well as permutation matrices as particular representations thereof. Finally, we come to the important notion of permutation cycles, which correspond to the conjugacy classes of the symmetric group. The following sections then deal with the mathematical description of systems of distinguishable and indistinguishable particles. From the defining relation for many-particle states we derive the explicit form of these in terms of states that are either completely symmetric or completely antisymmetric under the exchange of a pair of particles. Then, we review the continuous Fock-space representation of position eigenstates and thereafter the discrete, or occupation-number representation.

In Chapter 3, we develop the canonical and the grand-canonical description of ideal quantum gases. Beginning with a short review of ensembles of statistical mechanics, we turn to the one-particle time evolution amplitude, which represents the central quantity both in the canonical and the grand-canonical description. We then introduce Wick rotation, which connects quantum mechanics and statistical physics. By Wick rotation, the real-time evolution amplitude becomes the imaginary time one for which we derive a path-integral representation in the next subsection. In the following, we first turn to the grand-canonical description, for which we briefly motivate the Van-Vleck-Pauli-Morette formula. From this we then calculate the time-evolution amplitude of the harmonic oscillator, before we derive the harmonic oscillator's many-particle partition function, using the cycle decomposition of Chapter 2 with the permutations that appear in the (anti-)symmetrised many-particle states for bosons and fermions. We then pass to the more popular grand-canonical description, where we calculate the grand-canonical partition function.

In the second part of this thesis, which consists of Chapter 4, we present our results for the quench dynamics of harmonically trapped ideal quantum gases. To that end, we calculate in the canonical ensemble the effect of a quench of trap frequency for a single particle in a harmonic potential well. We find that the corresponding one-particle width factorises into the well-known thermodynamic width and a function which carries the time dependence. The latter oscillates with twice the frequency of the final harmonic potential. Repeating our calculations for the case of two particles, we obtain the time dependent density matrix and the two-particle partition function, as well as the time dependent reduced density matrix in this two-particle ensemble.

We then generalise to the case of N particles. We obtain an expression for the time dependent N-particle density matrix in terms of the sum over all permutations of a product of one-particle density matrices. In order to calculate the N-particle partition function, we explicitly integrate out all coordinate dependencies of the time dependent N-particle density matrix. In the corresponding multi-dimensional Gaussian integral, there appear permutation dependent matrices, which complicates the integration considerably. We obtain a general expression for their determinants by noting that, because of the decomposition of the permutation group into conjugacy classes, there is also a cycle decomposition of the determinant of the above permutation dependent matrices, with the same subdeterminant factor for every n-cycle. We proceed in the calculation of this cycle factor by Laplace expanding a suitable single-cycle matrix, obtaining a difference equation, which we solve via a Z-transform. This yields the well-known expression for the N-particle partition function in cycle reduced form.

Next, we calculate the time dependent reduced one-particle density matrix in an N-particle ensemble by performing a partial trace over $N-1$ particle coordinates, during which integrals over broken cycles appear. In order to deal with these, we derive a master equation for their corresponding contributions. From this we obtain the reduced one-particle width and we find that this quantity also factorises into a time dependent and a thermodynamic part. We discuss the behaviour of the reduced one-particle width for different ensemble particle numbers and derive an expression for their high-temperature asymptotes.

For comparison, we calculate the time-dependent grand-canonical density matrix and the corresponding reduced one-particle one, for which we obtain an expression in terms of a weighed sum of canonical one-particle density matrices.

Finally, Chapter 5 summarises the results of this thesis and Chapter 6 discusses further interesting problems in the realm of non-equilibrium quantum statistics.

Chapter 2

Many-Particle Quantum Statistics

As we will be mainly working in the canonical ensemble, where the time evolution amplitude is given by the expectation value of the Wick-rotated time evolution operator between many-particle states, it useful to review the quantum mechanical description of many-particle systems of distinguishable and indistinguishable particles. We start by giving an overview of the permutation group in section 2.1, focusing on its decomposition into conjugacy classes, from which follows a decomposition of permutations into cycles. The cycle structure of the symmetric group provides the fundamental tool for the mathematical description of the quantum statistics of ideal and weakly interacting quantum gases.

2.1 Permutations and Cycles

A permutation is a bijective map from a finite ordered set M, that contains every element only once, to itself [18]:

$$P\colon M \longrightarrow M \tag{2.1}$$

Practically, a permutation corresponds to a rearrangement of the elements of M: Consider the N-tuple (the ordered set, or sequence, of N elements) $S = (1, 2, 3, \dots, N)$. A permutation P rearranges the elements of S. For example, $P(S) = (2, 1, 3, \dots, N)$ is the permutation that interchanges the first two elements of S. A permutation that interchanges any two elements is called a transposition. Another example for a permutation on S is $P'(S) = (5, 3, 4, 2, 1, 6, 7, \dots, N)$ where the first five elements are involved. One method of writing a permutation is relation notation, where the original sequence or N-tuple is in the first line and the permuted sequence is written in the second line of a $(N \times 2)$ matrix. Thus, in relation notation, P and P' are written as

$$P(S) = \begin{pmatrix} 1 & 2 & 3 & 4 & \dots & N \\ 2 & 1 & 3 & 4 & \dots & N \end{pmatrix} , \qquad P'(S) = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 & 6 & 7 & \dots & N \\ 5 & 3 & 4 & 2 & 1 & 6 & 7 & \dots & N \end{pmatrix} . \tag{2.2}$$

In general, for a permutation P, $P(i)$ is the action of P on the i-th element of the original sequence S, given by

$$P(S) = \begin{pmatrix} i \\ P(i) \end{pmatrix} = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 & \dots & N \\ P(1) & P(2) & P(3) & P(4) & P(5) & \dots & P(N) \end{pmatrix} . \tag{2.3}$$

Any permutation P of a finite set S can be expressed as the composition (product) of transpositions P_{ij}:

$$P(S) = \prod_{i,j=1}^{N} P_{ij} . \tag{2.4}$$

Here the transposition P_{ij}, which is defined as

$$P_{ij}\left((1,\ldots,i,\ldots,j,\ldots)\right)=(1,\ldots,j,\ldots,i,\ldots)\ , \tag{2.5}$$

is the special two element interchanging permutation mentioned above. For a sequence S of N elements, there are in total $N!$ permutations. This can be seen quite easily as there are N possible choices for the first element of the sequence. Once the first element has been fixed, there are $(N-1)$ elements left in S, thus for the second element, there are $(N-1)$ possible choices, for the third element we have $(N-2)$ possible choices and so on. Consequently, for the first two elements, there are $N\times(N-1)$ possible choices, for the first three elements we have $N\times(N-1)\times(N-2)$, and for the full set of N elements there are $N!$ different choices, i.e. permutations.

There are different ways of enumerating permutations. In this thesis we employ lexicographic ordering, i.e. the permutations are listed in numeric or dictionary order. Permutation P precedes permutation P' in lexicographic order if and only if for the minimum value of index i such that $P(i)\neq P'(i)$, we have $P(i)<P'(i)$. For example, for $N=4$, the permutations in lexicographic order of $(1,2,3,4)$ are from top to bottom and right to left:

$$\begin{array}{llll}
P_1=(1,2,3,4) & P_7=(2,1,3,4) & P_{13}=(3,1,2,4) & P_{19}=(4,1,2,3)\\
P_2=(1,2,4,3) & P_8=(2,1,4,3) & P_{14}=(3,1,4,2) & P_{20}=(4,1,3,2)\\
P_3=(1,3,2,4) & P_9=(2,3,1,4) & P_{15}=(3,2,1,4) & P_{21}=(4,2,1,3)\\
P_4=(1,3,4,2) & P_{10}=(2,3,4,1) & P_{16}=(3,2,4,1) & P_{22}=(4,2,3,1)\\
P_5=(1,4,2,3) & P_{11}=(2,4,1,3) & P_{17}=(3,4,1,2) & P_{23}=(4,3,1,2)\\
P_6=(1,4,3,2) & P_{12}=(2,4,3,1) & P_{18}=(3,4,2,1) & P_{24}=(4,3,2,1)\ .
\end{array} \tag{2.6}$$

2.1.1 Symmetric Group S_N

Two permutations P and P' of a set M may be applied successively, i.e., $P\circ P'$, where the result is again a permutation. Thus, the set of permutations of M together with the operation of composition of permutations $\circ$ forms a group, called the *symmetric group* of degree N and denoted by $S_N=(M,\circ)$, so that

1. The identity element corresponds to the unpermuted set:

$$\mathbb{1}_{S_N}=\left(\begin{smallmatrix}1&2&3&\ldots&N\\1&2&3&\ldots&N\end{smallmatrix}\right)\in S_N\ . \tag{2.7}$$

2. The inverse corresponds to the inverse permutation:

$$P^{-1}=\begin{pmatrix}1&2&3&\ldots&N\\P(1)&P(2)&P(3)&\ldots&P(N)\end{pmatrix}^{-1}=\begin{pmatrix}P(1)&P(2)&P(3)&\ldots&P(N)\\1&2&3&\ldots&N\end{pmatrix}\ . \tag{2.8}$$

3. The operation $\circ$ is associative:

$$(P\circ P')\circ P''=P\circ(P'\circ P'')\qquad\text{for all}\qquad P,P',P''\in M\ . \tag{2.9}$$

Subgroups of S_N are called permutation groups. A permutation matrix is a square binary matrix, i.e. a matrix that has only entries of 0 and 1, with exactly one entry 1 in each row and each column and zeros elsewhere. The $(N \times N)$ permutation matrix $\mathbf{P}$ that corresponds to a permutation $P \in S_N$ is constructed by permuting the columns of the $(N \times N)$ identity matrix $\mathbb{1}_N$ according to P, i.e.

$$\mathbf{P}_P = (\delta_{i,P(j)}) = \left(\mathbf{e}_{P(1)}, \mathbf{e}_{P(2)}, \ldots, \mathbf{e}_{P(N)}\right) \ , \tag{2.10}$$

where $\mathbf{e}_i$ denotes the ith unit vector. Some examples for permutation matrices with $N = 4$ are:

$$\mathbf{P}_1 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \ , \qquad \mathbf{P}_{10} = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \end{pmatrix} \ , \qquad \mathbf{P}_{12} = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \ . \tag{2.11}$$

A *faithful representation* R of a group G is defined as a group isomorphism, i.e. a bijective map that preserves group structure, from G to a group of operators $R(G)$ on a linear vector space over some field $\mathbb{V}$, denoted $\mathrm{GL}(n, \mathbb{V})$ (the group of all linear operators of dimension n on $\mathbb{V}$), that is

$$g \ \in \ G \xrightarrow{R} R(G) \ \in \ \mathrm{GL}(n, \mathbb{V}) \ . \tag{2.12}$$

The representation matrices $R(G)$ thus obey the same multiplication rules as the original group elements. Specifically, for $g_1, g_2 \in G$ we have $R(g_1 \circ g_2) = R(g_1) \circ R(g_2)$, as well as $R(\mathbb{1}_G) = \mathbb{1}_{R(G)}$ and $R(g^{-1}) = R^{-1}(g_1)$.

It is straightforward to see that the map (2.10) is a faithful representation of S_N on a subgroup of $\mathrm{GL}(N, \mathbb{R})$, where the permutation matrices introduced above are the representation matrices of their corresponding permutation. It follows that, given the permutation matrix $\mathbf{P}_P$ of some permutation P, the inverse of $\mathbf{P}_P$ is the permutation matrix of the inverse permutation P^{-1}, that is $\mathbf{P}_P^{-1} = \mathbf{P}_{P^{-1}}$. Given permutations P and P' from S_N, the product of their corresponding permutation matrices $\mathbf{P}_P$ and $\mathbf{P}_{P'}$ is equal to the permutation matrix of the composite permutation $P \circ P'$:

$$\mathbf{P}_P \mathbf{P}_{P'} = \mathbf{P}_{P \circ P'} \ . \tag{2.13}$$

2.1.2 Permutation Cycles

There exists another essential notation for permutations. Let us take $N = 4$ and $P_{12} = \left(\begin{smallmatrix} 1 & 2 & 3 & 4 \\ 2 & 4 & 3 & 1 \end{smallmatrix}\right)$, which is the permutation that corresponds to the third matrix displayed in (2.11). P_{12} changes 1 to 2, then 2 to 4 and 4 back to 1 again. Additionally, 3 is left untouched, in other words 3 "is changed" to 3. For another permutation, e.g. for P_8 we have: $P_8 = \left(\begin{smallmatrix} 1 & 2 & 3 & 4 \\ 2 & 1 & 4 & 3 \end{smallmatrix}\right)$, that is, 1 is changed to 2 and then 2 goes back to 1 again. Then, 3 goes to 4 and 4 goes back to 3. We see that we can write the permutation in terms of how the elements change when the permutation is successively applied. This is called cycle notation, where the term *permutation cycle* or just *cycle* refers to a cyclic permutation of some or all elements of the permutation. In other words: A permutation cycle is a subset of a permutation whose elements trade places with one another in a cyclic fashion. Permutation cycles are sometimes called "orbits". For the example permutations above, we have $P_{12} = (3)(124)$, so P_{12} consists of a *one*-cycle and a *three*-cycle, and $P_8 = (12)(34)$ decomposes into two *two*-cycles. One-cycles, i.e. elements that are not changed by their respective permutation are also called *fixed points* and two-cycles are just transpositions.

P_n	Permuted sequence	Relation notation	Cycle notation
P_1	$(1,2,3)$	$\left(\begin{smallmatrix}1&2&3\\1&2&3\end{smallmatrix}\right)$	$(1)(2)(3)$
P_2	$(1,3,2)$	$\left(\begin{smallmatrix}1&2&3\\1&3&2\end{smallmatrix}\right)$	$(1)(2\,3)$
P_3	$(2,1,3)$	$\left(\begin{smallmatrix}1&2&3\\2&1&3\end{smallmatrix}\right)$	$(3)(1\,2)$
P_4	$(2,3,1)$	$\left(\begin{smallmatrix}1&2&3\\0&1&0\end{smallmatrix}\right)$	$(1\,2\,3)$
P_5	$(3,1,2)$	$\left(\begin{smallmatrix}1&2&3\\0&1&0\end{smallmatrix}\right)$	$(1\,3\,2)$
P_6	$(3,2,1)$	$\left(\begin{smallmatrix}1&2&3\\0&1&0\end{smallmatrix}\right)$	$(2)(1\,3)$

Table 2.1: All permutations of (123), i.e. all elements of S_3 in relation notation and cycle notation.

Every permutation in S_N decomposes into a product of disjoint cycles; this representation is unique up to the order of the factors. However, there is a great deal of freedom in picking the representation of a cyclic decomposition. In addition to the freedom in choosing the ordering of cycles, any rotation of a given cycle specifies the same cycle, so we could also have written $P_{12} = (3)(124) = (124)(3) = (241)(3) = (3)(412)$ and $P_8 = (12)(34) = (34)(12) = (43)(21)$, etc. Therefore it is customary to fix a notation by sorting the cycle representation of a given permutation in lowest canonical order, i.e. first by cycle length, and then by lowest initial order of elements within each cycle. Table 2.1 displays the elements of S_3, i.e. all permutations of the sequence $(1,2,3)$ in different notations.

We obtain the inverse of some permutation in cycle notation by leaving the first element and reversing the order of the other elements for every cycle, so we get $P_{12}^{-1} = (3)(142)$ and $P_8^{-1} = (12)(34)$ as well as $P_{10}^{-1} = \left(\begin{smallmatrix}1&2&3&4\\4&1&2&3\end{smallmatrix}\right)^{-1} = (1234)^{-1} = (1432)$.

The elements of any group G may be partitioned into conjugacy classes where members of the same conjugacy class have many properties in common. Two elements a and b of G are called conjugate $a \sim b$, if there exists an element g in G with

$$g^{-1}\,a\,g = b\,. \tag{2.14}$$

It is easy to see that the relation $\sim$ is reflexive, i.e., $a \sim a$, symmetric, i.e., $a \sim b \Leftrightarrow b \sim a$, and transitive, i.e. if $a \sim b$ and $b \sim c$ then $a \sim c$, so conjugacy is an equivalence relation and therefore partitions G into equivalence classes. This means that every element of the group belongs to precisely one conjugacy class, and the classes $\mathrm{Cl}(a)$ and $\mathrm{Cl}(b)$ are equal if and only if a and b are conjugate, and disjoint otherwise.

The conjugacy classes of S_N correspond to the cycle structures of permutations; that is, two elements of S_N are conjugate in S_N if and only if they consist of the same number of disjoint cycles of the same lengths. For example, taking $N = 4$ again, $P_9 = (4)(123)$ and $P_{12} = (3)(124)$ are conjugate; $P_1 = (1)(2)(3)(4)$ and $P_8 = (12)(34)$ are not. Specifically, the identity element $\mathbb{1}_G$ of a group G, i.e. P_1 for S_N is always in its own class.

Of course, conjugacy has its counterpart in the representation group $R(G)$, where it is called *similarity.* Two $(N \times N)$ matrices A and B in $R(G)$ are called similar if for some representation matrix C we have

$$C^{-1}\,A\,C = B\,. \tag{2.15}$$

Similar matrices share many properties, for example:

- rank

- determinant
- trace
- eigenvalues
- characteristic polynomial

etc., since they are related by an orthogonal similarity transformation, i.e. they represent the same linear transformation under two different bases, with C being the change of base matrix.

Thus, two permutation matrices, where the corresponding permutations have the same cycle structure, i.e. the same number of cycles with the same lengths, are similar.

2.2 Distinguishable Particles

Particles are called distinguishable, if they can be distinguished in terms of some measurable property. Consequently, distinguishable particles can be enumerated and the mathematical formalism for their description follows readily from a generalisation of the postulates of one-particle quantum mechanics to the case of an N-particle quantum system. In order to describe a quantum mechanical system, one first has to specify the Hilbert space, that the system's state lives in. Secondly, one constructs a set of states that form a basis in the respective Hilbert space.

For an N-particle system the space that the corresponding states live in can be constructed as a direct product of one-particle Hilbert spaces $\mathcal{H}_1$. Let $\mathcal{H}_1^{(i)}$ denote the Hilbert space of the ith particle, then the multiparticle Hilbert space for the whole N-particle system is

$$\mathcal{H}_N = \mathcal{H}_1^{(1)} \otimes \mathcal{H}_1^{(2)} \otimes \cdots \otimes \mathcal{H}_1^{(N)} \ . \tag{2.16}$$

The elements of $\mathcal{H}_N$ are N-particle states that are themselves a tensor product of one-particle states $|\varphi\rangle$, such that the ith particle with one-particle state $|\varphi_i\rangle$ lives in the ith one-particle Hilbert space $\mathcal{H}_1^{(i)}$, where the symbol φ stands for all quantum numbers that characterise the particle. The N-particle states thus read

$$|\varphi^{(N)}\rangle = |\varphi_1\varphi_2\cdots\varphi_N\rangle = |\varphi_1\rangle|\varphi_2\rangle\cdots|\varphi_N\rangle = |\varphi_1\rangle \otimes |\varphi_2\rangle \otimes \cdots \otimes |\varphi_N\rangle \ . \tag{2.17}$$

Let $\{\hat{O}^{(i)}\}$ be a complete set of commuting observables in $\mathcal{H}_1^{(i)}$, then the corresponding eigenstates $\{|\varphi_{\mathrm{e}}^{(i)}\rangle\}$ form a basis of $\mathcal{H}_1^{(i)}$. We may assume these to be orthonormal:

$$\langle\varphi_\alpha^{(i)}\,|\,\varphi_\beta^{(i)}\rangle = \begin{cases} \delta_{\alpha\beta} & \text{discrete basis} \\ \delta(\alpha-\beta) & \text{continuous basis .} \end{cases} \tag{2.18}$$

Consequently, a basis of $\mathcal{H}_N$ is constructed by taking the direct product of the corresponding single-particle basis states $|\varphi^{(N)}\rangle = |\varphi_{\alpha_1}^{(1)}\rangle|\varphi_{\alpha_2}^{(2)}\rangle\cdots|\varphi_{\alpha_N}^{(N)}\rangle$. A general N-particle state $|\psi_N\rangle$ can be expanded in terms of the $|\varphi^{(N)}\rangle$:

$$|\psi_N\rangle = \sum_{\alpha_i} C(\alpha_1,\alpha_2,\ldots,\alpha_N)|\varphi_{\alpha_1}^{(1)}\rangle|\varphi_{\alpha_2}^{(2)}\rangle\cdots|\varphi_{\alpha_N}^{(N)}\rangle \ . \tag{2.19}$$

The same statistical interpretation holds for an N-particle state as for a single-particle state: Therefore, $|C(\alpha_1,\alpha_2,\ldots,\alpha_N)|^2$ represents the probability for a measurement of the observable $\hat{O}$ in the state $|\psi_N\rangle$ to yield the eigenvalue of $\hat{O}$, i.e. $|\varphi_{\alpha_1}^{(1)}\rangle|\varphi_{\alpha_2}^{(2)}\rangle\cdots|\varphi_{\alpha_N}^{(N)}\rangle$.

2.3 Identical Particles

In reality, the only observable properties, that a quantum mechanical particle like an electron has, are its quantum numbers, which are the eigenvalues of an associated observable, i.e. an Hermitian operator. It follows, that quantum particles, which have similar or equal values for all of their quantum numbers, cannot, in principle, be distinguished. As an example for particles that share the same quantum numbers, consider the fraction of particles of an ideal quantum gas, which is in its ground state. If the gas is confined to an harmonic trap, the particles in the ground state will share the same volume at the trap's potential minimum, thus their wavefunctions will overlap.

Thus, when dealing with multiparticle quantum systems, we must take into account the *principle of indistinguishability* and consequently, every physical problem, which requires the observation of single particles, must be regarded as physically meaningless for systems of identical particles. Now, for computational reasons, an enumeration of particles is unavoidable, since we must be able to enumerate the system's one-particle states. However, this enumeration must be carried out in such a way, that above principle is respected, i.e. that physically relevant quantities are invariant with respect to changes in the enumeration scheme. Otherwise it would be possible to perform a measurement which could in principle distinguish between particles.

The only physically relevant properties are the expectation values of observables. Therefore, the relation

$$\langle\varphi_1\cdots\varphi_i\cdots\varphi_j\cdots\varphi_N|\,\hat{O}\,|\varphi_1\cdots\varphi_i\cdots\varphi_j\cdots\varphi_N\rangle = \langle\varphi_1\cdots\varphi_j\cdots\varphi_i\cdots\varphi_N|\,\hat{O}\,|\varphi_1\cdots\varphi_j\cdots\varphi_i\cdots\varphi_N\rangle \tag{2.20}$$

may be regarded as the defining equation for the states of systems of identical particles. On the right side of (2.20), the coordinates of particles i and j are permuted with respect to those on the left. We now ask if there is an operator $\hat{P}_{ij}$ which, when applied to a state, interchanges coordinates in the above way. Of course, the right side of (2.20) differs from the left side by a transposition (2.5) and the operator in question is the *transposition operator*, which we define as

$$\hat{P}_{ij}|\varphi_1\cdots\varphi_i\cdots\varphi_j\cdots\varphi_N\rangle = |\varphi_1\cdots\varphi_j\cdots\varphi_i\cdots\varphi_N\rangle\ . \tag{2.21}$$

Before going on, let us review some of the properties of the transposition operator. Applying $\hat{P}_{ij}$ to an N-particle state twice obviously yields the initial state. This means that

$$\hat{P}_{ij}^2 = \hat{\mathbb{1}} \quad\Longleftrightarrow\quad \hat{P}_{ij} = \hat{P}_{ij}^{-1}\ , \tag{2.22}$$

so $\hat{P}_{ij}$ is an involution, i.e. it is self-inverse. Equation (2.20), which is written in coordinate representation can now be rewritten in the following coordinate independent form:

$$\langle\varphi^{(N)}|\,\hat{O}\,|\varphi^{(N)}\rangle = \langle\hat{P}_{ij}\varphi^{(N)}|\,\hat{O}\,|\hat{P}_{ij}\varphi^{(N)}\rangle = \langle\varphi^{(N)}|\,\hat{P}_{ij}^{\dagger}\hat{O}\hat{P}_{ij}\,|\varphi^{(N)}\rangle\ . \tag{2.23}$$

We should stress that this holds for arbitrary N-particle states in $\mathcal{H}_N$ and also for all matrix elements of the type $\langle\varphi^{(N)}|\,\hat{O}\,|\psi^{(N)}\rangle$, since these are trivially brought into the above form by the decomposition

$$\langle\varphi^{(N)}|\,\hat{O}\,|\psi^{(N)}\rangle = \frac{1}{4}\Big\{\langle\varphi^{(N)}+\psi^{(N)}|\,\hat{O}\,|\varphi^{(N)}+\psi^{(N)}\rangle - \langle\varphi^{(N)}-\psi^{(N)}|\,\hat{O}\,|\varphi^{(N)}-\psi^{(N)}\rangle \\ + i\langle\varphi^{(N)}+i\psi^{(N)}|\,\hat{O}\,|\varphi^{(N)}+i\psi^{(N)}\rangle - i\langle\varphi^{(N)}-i\psi^{(N)}|\,\hat{O}\,|\varphi^{(N)}-i\psi^{(N)}\rangle\Big\}\ . \tag{2.24}$$

This leads to the operator identity

$$\hat{O} = \hat{P}_{ij}^{\dagger}\hat{O}\hat{P}_{ij} \qquad \text{for all} \quad i,j\ . \tag{2.25}$$

Thus, it is a necessary precondition for the observables of a system of indistinguishable i.e. identical particles, that they depend explicitly on the coordinates of all N particles. If in (2.25) we make the particular choice $\hat{O} = \hat{\mathbb{1}}$ for the observable, we get by applying (2.22)

$$\hat{\mathbb{1}} = \hat{P}_{ij}^{\dagger}\hat{P}_{ij} \quad \Longrightarrow \quad \hat{P}_{ij} = \hat{P}_{ij}^{\dagger}\hat{P}_{ij}^{2} = \hat{P}_{ij}^{\dagger}\ ; \tag{2.26}$$

thus, the transposition operator $\hat{P}_{ij}$ is both Hermitian and unitary:

$$\hat{P}_{ij} = \hat{P}_{ij}^{\dagger} \quad , \qquad \hat{P}_{ij}^{\dagger} = \hat{P}_{ij}^{-1}\ . \tag{2.27}$$

It also follows from (2.25), that

$$\hat{P}_{ij}\hat{O} = \hat{P}_{ij}\hat{P}_{ij}^{\dagger}\hat{O}\hat{P}_{ij} = \hat{O}\hat{P}_{ij}\ , \tag{2.28}$$

which means that all observables of the N-particle system commute with $\hat{P}_{ij}$:

$$\big[\hat{P}_{ij},\hat{O}\big]_{-} = \hat{P}_{ij}\hat{O} - \hat{O}\hat{P}_{ij} \equiv 0\ , \tag{2.29}$$

in particular the Hamiltonian, which generates the system's time evolution, i.e.

$$\big[\hat{P}_{ij},\hat{H}\big]_{-} = 0\ . \tag{2.30}$$

According to the principle of indistinguishability for identical particles, an N-particle state $|\psi_N\rangle$ may only change in terms of a phase factor under the action of $\hat{P}_{ij}$. Consequently, $|\psi_N\rangle$ must be an eigenstate of $\hat{P}_{ij}$:

$$\hat{P}_{ij}|\varphi_1\cdots\varphi_i\cdots\varphi_j\cdots\varphi_N\rangle = |\varphi_1\cdots\varphi_j\cdots\varphi_i\cdots\varphi_N\rangle \overset{!}{=} \lambda|\varphi_1\cdots\varphi_i\cdots\varphi_j\cdots\varphi_N\rangle\ , \tag{2.31}$$

and because of the unitarity and involutory properties (2.27) and (2.22) of the transposition operator, $\hat{P}_{ij}$ has only the real eigenvalues of $\lambda = \pm 1$, which are independent of the particular pair i,j. It follows that

> the states of a system of identical particles are either completely *symmetric* or completely *antisymmetric* under exchange of a pair of particles.

Because of (2.30), we have $[\hat{P}_{ij},\hat{U}(t)] = 0$, so $\hat{P}_{ij}$ commutes with the time evolution operator

$$\hat{U}(t-t_0) = \exp\left\{-\frac{i}{\hbar}\hat{H}(t-t_0)\right\} \tag{2.32}$$

and, accordingly, the states of a system of N identical particles retain their symmetry character for all times. Thus, the Hilbert space $\mathcal{H}_N$ of a system of N identical particles decomposes into

$\mathcal{H}_N^{(+)}$: the Hilbert space of symmetric states $|\varphi_N^{(+)}\rangle$:

$$\hat{P}_{ij}|\varphi_N^{(+)}\rangle = |\varphi_N^{(+)}\rangle \tag{2.33}$$

$\mathcal{H}_N^{(-)}$: the Hilbert space of antisymmetric states $|\varphi_N^{(-)}\rangle$:

$$\hat{P}_{ij}|\varphi_N^{(-)}\rangle = -|\varphi_N^{(-)}\rangle \; . \tag{2.34}$$

We may combine both cases by writing $\hat{P}_{ij}|\varphi_N^{(\epsilon)}\rangle = \epsilon|\varphi_N^{(\epsilon)}\rangle$, where we use $\epsilon = +1$ for symmetric and $\epsilon = -1$ for antisymmetric states. Symmetric and antisymmetric states are orthogonal to each other:

$$\langle\varphi_N^{(-)}|\varphi_N^{(+)}\rangle = \langle\varphi_N^{(-)}|\hat{P}_{ij}\varphi_N^{(+)}\rangle = \langle\hat{P}_{ij}\varphi_N^{(-)}|\varphi_N^{(+)}\rangle = -\langle\varphi_N^{(-)}|\varphi_N^{(+)}\rangle = 0 \; . \tag{2.35}$$

We are now in the position to ask ourselves, how an (anti-)symmetrized N-particle state $|\varphi_N^{(\epsilon)}\rangle$ is constructed. To answer this question, we may start with a non-symmetrized N-particle state (2.19), which has now to be symmetrized or anti-symmetrized in a suitable way. To achieve this, we may define a symmetrization operator

$$\hat{S}_\epsilon = \sum_P \epsilon^{p(P)} \hat{P}(P) \; , \tag{2.36}$$

where we have introduced the permutation operator, which is given as a suitable product of transposition operators [recall (2.4)]

$$\hat{P}(P) = \prod_{i,j=1}^{N} \hat{P}_{ij} \; , \tag{2.37}$$

and which acts on multi-particle states by permuting the particles according to the permutation P:

$$\hat{P}(P)|\varphi_1\varphi_2\cdots\varphi_N\rangle = |\varphi_{P(1)}\varphi_{P(2)}\cdots\varphi_{P(N)}\rangle \; . \tag{2.38}$$

The sum in (2.36) runs over all permutations P and $p(P)$ denotes the number of transpositions that construct the current permutation via equation (2.37). It can be shown [24] that the N-particle states of identical particles can be only of the type $|\varphi_N^{(\pm)}\rangle$ and that they retain their symmetry character for all times. Thus, we can state:

> The states of a system of N identical particles either all belong to $\mathcal{H}_N^{(+)}$, or else they all belong to $\mathcal{H}_N^{(-)}$.

Which space, $\mathcal{H}_N^{(+)}$ or $\mathcal{H}_N^{(-)}$, is the right one for which type of particle can be found in relativistic quantum field theory. In 1940 W. Pauli proved the so-called *spin-statistics theorem* [23], a critical result of quantum field theory which states that particles with half-integer spin are fermions, while particles with integer spin are bosons, i.e.:

- $\mathcal{H}_N^{(+)}$ is the space of the *symmetric* state of N identical particles of **integer spin**. These are called **bosons**.

- $\mathcal{H}_N^{(-)}$ is the space of the *antisymmetric* state of N identical particles of **half-integer spin**. These are called **fermions**.

In the following two sections we will introduce creation and annihilation operators, which arise in the field-theoretic description of many-particle quantum systems, that is also known as "second quantisation", despite the fact that this is somewhat of a misnomer.

Our first task along this way consists in constructing a basis for the space $\mathcal{H}_N^{(\epsilon)}$ using appropriate single-particle states $|\varphi_i\rangle$. In the process, we must distinguish the cases in which the associated single-particle observable $\hat{\varphi}_i$ has a discrete or a continuous spectrum.

2.3.1 Continuous Fock Space of Position Eigenstates

In this section we first discuss the case of a *continuous* single-particle spectrum. This will lead us to the continuous Fock space of position eigenstates.

Let $\hat{\varphi}$ be a single-particle observable with a continuous spectrum:

$$\hat{\varphi}|\varphi_\alpha\rangle = \varphi_\alpha|\varphi_\alpha\rangle \ , \qquad \text{with} \qquad \langle\varphi_\alpha\,|\,\varphi_\beta\rangle = \delta(\alpha-\beta) \ . \tag{2.39}$$

The eigenstates are assumed to form an orthonormal basis of $\mathcal{H}_1$:

$$\int d\varphi_\alpha|\varphi_\alpha\rangle\langle\varphi_\alpha| = \mathbb{1} \ . \tag{2.40}$$

A non-symmetrised N-particle state (2.19) is then given by

$$|\varphi_{1\alpha}\cdots\varphi_{N\alpha}\rangle = |\varphi_{1\alpha}\rangle|\varphi_{2\alpha}\rangle\ldots|\varphi_{N\alpha}\rangle \ . \tag{2.41}$$

where the first index refers to the particle and the αs in the second index are complete sets of quantum numbers. Here, we should add a comment on our convention regarding indices. As — for typographical reasons — we want to avoid sub-subscripts, as e.g., in φ_{α_1}, we have adopted the following notation: The first index in $\varphi_{i\alpha}$, i.e. i, is the particle index and the second index, α, denotes the complete set of quantum numbers of the ith particle. Thus, $\varphi_{1\alpha} \equiv \varphi_{\alpha_1}$ and if we print the quantum numbers alone, as in $\delta(\beta-\alpha_i)$, we put an index i, corresponding to the particle number.

The single-particle states in (2.41) are ordered arbitrarily, but in some well-defined way. Application of the symmetrisation operator (2.36) to (2.41) then yields the (anti-)symmetrised N-particle state

$$\begin{aligned}|\varphi_{1\alpha}\cdots\varphi_{N\alpha}\rangle^{(\epsilon)} &= \frac{1}{N!}\sum_P \epsilon^{p(P)}\hat{P}(P)|\varphi_{1\alpha},\ldots,\varphi_{N\alpha}\rangle \\ &= \frac{1}{N!}\sum_P \epsilon^{p(P)}|\varphi_{P(1)\alpha},\ldots,\varphi_{P(N)\alpha}\rangle \ , \end{aligned} \tag{2.42}$$

with the normalisation factor $1/N!$. Note, that in (2.42) we have used the superscript ϵ to indicate that the corresponding expression is (anti-) symmetrized, and we will stick with this notation throughout the present thesis. It is straightforward to show that the permutation operator is Hermitian by taking the expectation value of its Hermitian conjugate:

$$\langle\psi_N^{(\epsilon)}|\,\hat{P}^\dagger(P)\,|\varphi_N^{(\epsilon)}\rangle = \left(\langle\varphi_N^{(\epsilon)}|\,\hat{P}(P)\,|\psi_N^{(\epsilon)}\rangle\right)^* = \epsilon^{p(P)}\left(\langle\varphi_N^{(\epsilon)}\,|\,\psi_N^{(\epsilon)}\rangle\right)^* \tag{2.43}$$

$$= \epsilon^{p(P)}\langle\varphi_N^{(\epsilon)}\,|\,\psi_N^{(\epsilon)}\rangle = \langle\varphi_N^{(\epsilon)}|\,\hat{P}(P)\,|\psi_N^{(\epsilon)}\rangle \ , \tag{2.44}$$

where we have used the eigenvalue equation of the permutation operator

$$\hat{P}(P)|\psi_N^{(\epsilon)}\rangle = \epsilon^{p(P)}|\psi_N^{(\epsilon)}\rangle\,, \tag{2.45}$$

which follows from the definition of the symmetrisation operator (2.36). Thus we have $\hat{P}(P) = \hat{P}^\dagger(P)$ in $\mathcal{H}_N^{(\epsilon)}$ and we are now prepared to calculate the expectation value of an arbitrary observable $\hat{A}$ between the (anti-)symmetrised states (2.42):

$$\begin{aligned} &{}^{(\epsilon)}\langle\psi_{1\alpha}\cdots\psi_{N\alpha}|\,\hat{A}\,|\varphi_{1\beta}\cdots\varphi_{N\beta}\rangle^{(\epsilon)} \\ &\qquad = \left(\frac{1}{N!}\right)^2 \sum_{P'}\sum_{P''} \epsilon^{p(P')+p(P'')}\langle\psi_{1\alpha}\cdots\psi_{N\alpha}|\,\hat{P}^\dagger(P'')\hat{A}\hat{P}(P')\,|\varphi_{1\beta}\cdots\varphi_{N\beta}\rangle\,. \end{aligned} \tag{2.46}$$

Here, we may first interchange $\hat{P}^\dagger(P'')$ and $\hat{A}$ as, according to (2.29) and (2.37), the permutation operator also commutes with every allowed observable in $\mathcal{H}_N^{(\epsilon)}$. Secondly, it is obvious that the permutation operator inherits the composition law of the symmetric group, so it holds that $\hat{P}^\dagger(P'')\hat{P}(P') = \hat{P}(P)$ and we may define a composite permutation $\hat{P}(P)$, for which clearly we have $\epsilon^{p(P')+p(P'')} = \epsilon^{p(P)}$. Because there are only $N!$ distinct permutations in S_N, $N!$ terms in the double sum of (2.46) are superfluous, and we obtain

$$\begin{aligned} {}^{(\epsilon)}\langle\psi_{1\alpha}\cdots\psi_{N\alpha}|\,\hat{A}\,|\varphi_{1\beta}\cdots\varphi_{N\beta}\rangle^{(\epsilon)} &= \frac{1}{N!}\sum_P \epsilon^{p(P)}\langle\psi_{1\alpha}\cdots\psi_{N\alpha}|\,\hat{A}\hat{P}(P)\,|\varphi_{1\beta}\cdots\varphi_{N\beta}\rangle && (2.47)\\ &= \frac{1}{N!}\sum_P \epsilon^{p(P)}\langle\psi_{1\alpha}\cdots\psi_{N\alpha}|\,\hat{A}\,|\varphi_{P(1)\beta}\cdots\varphi_{P(N)\beta}\rangle && (2.48)\\ &= \frac{1}{N!}\sum_P \epsilon^{p(P)}\langle\psi_{P(1)\alpha}\cdots\psi_{P(N)\alpha}|\,\hat{A}\,|\varphi_{1\beta}\cdots\varphi_{N\beta}\rangle\,. && (2.49) \end{aligned}$$

The last equation (2.49) results if we interchange $\hat{P}(P')$ and $\hat{A}$ instead, so only the left state in the expectation value of (2.46) is (anti-)symmetrised. The above relation holds in particular when $\hat{A}$ is the identity operator $\hat{\mathbb{1}}$, so the scalar product of two (anti-)symmetrised many-particle states reads:

$$\begin{aligned} {}^{(\epsilon)}\langle\psi_{1\alpha}\cdots\psi_{N\alpha}\,|\,\varphi_{1\beta}\cdots\varphi_{N\beta}\rangle^{(\epsilon)} &= \frac{1}{N!}\sum_P \epsilon^{p(P)}\langle\psi_{1\alpha}\cdots\psi_{N\alpha}\,|\,\varphi_{P(1)\beta}\cdots\varphi_{P(N)\beta}\rangle && (2.50)\\ &= \frac{1}{N!}\sum_P \epsilon^{p(P)}\langle\psi_{P(1)\alpha}\cdots\psi_{P(N)\alpha}\,|\,\varphi_{1\beta}\cdots\varphi_{N\beta}\rangle\,. && (2.51) \end{aligned}$$

This may also be explicitly written in terms of the tensor product of one-particle states as in (2.19) and yields the orthonormalisation condition for (anti-)symmetrised N-particle states:

$$\begin{aligned} {}^{(\epsilon)}\langle\psi_{1\alpha}\cdots\psi_{N\alpha}\,|\,\varphi_{1\beta}\cdots\varphi_{N\beta}\rangle^{(\epsilon)} &= \frac{1}{N!}\sum_P \epsilon^{p(P)}\langle\psi_{1\alpha}\,|\,\varphi_{P(1)\beta}\rangle\cdots\langle\psi_{N\alpha}\,|\,\varphi_{P(N)\beta}\rangle && (2.52)\\ &= \frac{1}{N!}\sum_P \epsilon^{p(P)}\delta(\alpha_1-\beta_{P(1)})\cdots\delta(\alpha_N-\beta_{P(N)})\,. && (2.53) \end{aligned}$$

From (2.52) we can easily find a completeness relation by multiplying it with a ket from the left and subsequent integration over the continuous quantum numbers $i\alpha$. We get

$$\int \cdots \int d\alpha_1 \cdots d\alpha_N \, |\varphi_{1\alpha} \cdots \varphi_{N\alpha}\rangle^{(\epsilon)(\epsilon)} \langle \psi_{1\alpha} \cdots \psi_{N\alpha} | \varphi_{1\beta} \cdots \varphi_{N\beta}\rangle^{(\epsilon)} = |\varphi_{1\beta} \cdots \varphi_{N\beta}\rangle^{(\epsilon)} \tag{2.54}$$

due to (2.53) and from this we read off the completeness relation for the (anti-)symmetrised N-particle states in $\mathcal{H}_N^{(\epsilon)}$:

$$\int \cdots \int d\alpha_1 \cdots d\alpha_N \, |\varphi_{1\alpha} \cdots \varphi_{N\alpha}\rangle^{(\epsilon)} \langle \psi_{1\alpha} \cdots \psi_{N\alpha}|^{(\epsilon)} \, . \tag{2.55}$$

The states defined in (2.42) thus form a complete, orthonormalised basis in $\mathcal{H}_N^{(\epsilon)}$.

The above considerations make it clear how tedious it can be to work with (anti-)symmetrised N-particle states. We would thus like to find a way to construct these with the aid of special creation operators directly from the so-called vacuum state $|0\rangle$, which is the normalised many-particle state where no particles are present. This operator $\hat{b}_\beta^\dagger$ has the characteristic effect of linking many-particle Hilbert spaces of different numbers of particles to one another:

$$\hat{b}_\beta^\dagger : \mathcal{H}_N^{(\epsilon)} \to \mathcal{H}_{N+1}^{(\epsilon)} \, . \tag{2.56}$$

This *creation operator* is thus a particle number changing operator. It is defined by its action on (anti-)symmetrised states,

$$\hat{b}_\beta^\dagger \underbrace{|\varphi_{1\alpha} \cdots \varphi_{N\alpha}\rangle^{(\epsilon)}}_{\in \mathcal{H}_N^{(\epsilon)}} = \sqrt{N+1} \, \underbrace{|\varphi_\beta \varphi_{1\alpha} \cdots \varphi_{N\alpha}\rangle^{(\epsilon)}}_{\in \mathcal{H}_{N+1}^{(\epsilon)}} \, , \tag{2.57}$$

thus one can say that it *creates* an additional particle in the single-particle state $|\varphi_\beta\rangle$. The notation for the resulting $(N+1)$-particle state in (2.57) needs some explanation: Conventionally, the symbol for the newly created additional one-particle state φ_β is simply added at the left of the other symbols $\varphi_{1\alpha} \cdots \varphi_{N\alpha}$ that describe the previous N-particle state.

The other way round, we may create an arbitrary (anti-)symmetrised N-particle state by letting N creation operators act on the vacuum state. This reads

$$|\varphi_{1\alpha} \cdots \varphi_{N\alpha}\rangle^{(\epsilon)} = \frac{1}{\sqrt{N!}} \, \hat{b}_{1\alpha}^\dagger \hat{b}_{2\alpha}^\dagger \cdots \hat{b}_{N\alpha}^\dagger |0\rangle \, . \tag{2.58}$$

Here, it is crucial to observe the order of the operators, as interchanging two creation operators in (2.58) yields an additional factor ϵ:

$$\hat{b}_{1\alpha}^\dagger \hat{b}_{2\alpha}^\dagger |\varphi_{3\alpha} \cdots \varphi_{N\alpha}\rangle^{(\epsilon)} = \sqrt{N(N-1)} \, |\varphi_{1\alpha}\varphi_{2\alpha}\varphi_{3\alpha} \cdots \varphi_{N\alpha}\rangle^{(\epsilon)} \tag{2.59}$$

in contrast to

$$\hat{b}_{2\alpha}^\dagger \hat{b}_{1\alpha}^\dagger |\varphi_{3\alpha} \cdots \varphi_{N\alpha}\rangle^{(\epsilon)} = \epsilon \sqrt{N(N-1)} \, |\varphi_{1\alpha}\varphi_{2\alpha}\varphi_{3\alpha} \cdots \varphi_{N\alpha}\rangle^{(\epsilon)} \, , \tag{2.60}$$

where in (2.60) we have exchanged the symbols $\varphi_{1\alpha}$ and $\varphi_{2\alpha}$, to adapt the ket there to the one in (2.59). From these two equations, we find the commutator of two creation operators for bosons and fermions:

$$\left[\hat{b}_{1\alpha}^\dagger, \hat{b}_{2\alpha}^\dagger\right]_{-\epsilon} = \hat{b}_{1\alpha}^\dagger \hat{b}_{2\alpha}^\dagger - \epsilon \, \hat{b}_{2\alpha}^\dagger \hat{b}_{1\alpha}^\dagger = 0 \, . \tag{2.61}$$

These anticommute for fermions ($\epsilon = -1$) and commute for bosons ($\epsilon = +1$). If there is a creation operator, there must also be an *annihilation operator*, which links the Hilbert spaces $\mathcal{H}_N^{(\epsilon)}$ and $\mathcal{H}_{N-1}^{(\epsilon)}$ to one another, i.e.

$$\hat{b}_\alpha : \mathcal{H}_N^{(\epsilon)} \to \mathcal{H}_{N-1}^{(\epsilon)} \,. \tag{2.62}$$

Its action on (anti-)symmetrised states (2.42) can be found e.g. by computing the expectation value ${}^{(\epsilon)}\langle\varphi_{2\beta}\cdots\varphi_{N\beta}|\,\hat{b}_\gamma\,|\varphi_{1\alpha}\cdots\varphi_{N\alpha}\rangle^{(\epsilon)}$ (see Ref. [24]):

$$\begin{aligned}\hat{b}_\gamma|\varphi_{1\alpha}\cdots\varphi_{N\alpha}\rangle^{(\epsilon)} = \frac{1}{\sqrt{N}}\Big\{\, & \delta(\gamma-\alpha_1)\,|\varphi_{2\alpha}\cdots\varphi_{N\alpha}\rangle^{(\epsilon)} \\ & + \epsilon\,\delta(\gamma-\alpha_2)\,|\varphi_{1\alpha}\varphi_{3\alpha}\cdots\varphi_{N\alpha}\rangle^{(\epsilon)} \\ & \vdots \\ & + \epsilon^{N-1}\,\delta(\gamma-\alpha_N)\,|\varphi_{1\alpha}\cdots\varphi_{(N-1)\alpha}\rangle^{(\epsilon)}\Big\} \,. \end{aligned} \tag{2.63}$$

Thus, if the single-particle state $|\varphi_\gamma\rangle$ is present in the N-particle state $|\varphi_{1\alpha}\cdots\varphi_{N\alpha}\rangle^{(\epsilon)}$, application of the annihilation operator $\hat{b}_\gamma$ yields an $(N-1)$-particle state where $|\varphi_\gamma\rangle$ has been removed. Consequently, one says that $\hat{b}_\gamma$ *annihilates* a particle in state $|\varphi_\gamma\rangle$. If, however, $|\varphi_\gamma\rangle$ does not occur within the (anti-)symmetrised initial state, then the application of $\hat{b}_\gamma$ causes the initial state to vanish, i.e. the resulting state is the zero ket $|0\rangle$. An important special case is the annihilation of the vacuum state, where have:

$$\hat{b}_\gamma\,|0\rangle = 0 \,. \tag{2.64}$$

The (anti-)commutation relation for the annihilation operator then follows from (2.61):

$$\big[\,\hat{b}_{1\alpha}, \hat{b}_{2\alpha}\big]_{-\epsilon} = -\epsilon\left([\,\hat{b}^\dagger_{1\alpha}, \hat{b}^\dagger_{2\alpha}]_{-\epsilon}\right)^\dagger = 0 \,. \tag{2.65}$$

As in the commutation relation for the creation operators, the annihilation operators anticommute for fermions ($\epsilon = -1$) and commute for bosons ($\epsilon = +1$). We still have to find the third commutation relation for creation and annihilation operators, namely the mixed one, which specifies the (anti-) commutator between an annihilation and a creation operator (again, the proof can be found in Ref. [24]):

$$\big[\,\hat{b}_{1\alpha}, \hat{b}^\dagger_{2\alpha}\big]_{-\epsilon} = \delta(\alpha_1-\alpha_2) \,, \tag{2.66}$$

so they (anti-)commute in the case that the operators create and annihilate different particles. In the case that they create and annihilate the same particle, however, the (anti-)commutator yields one.

We will now introduce two more operators, which are essential for the description of many-particle quantum systems. One is the so-called *occupation-density operator*

$$\hat{n}_\alpha = \hat{b}^\dagger_\alpha \hat{b}_\alpha \,, \tag{2.67}$$

the eigenstates of which are the basis states of $\mathcal{H}_N^{(\epsilon)}$, so we have the following eigen equation,

$$\hat{n}_\beta\,|\varphi_{1\alpha}\cdots\varphi_{N\alpha}\rangle^{(\epsilon)} = \left[\sum_{i=1}^{n}\delta(\beta-\alpha_i)\right]|\varphi_{1\alpha}\cdots\varphi_{N\alpha}\rangle^{(\epsilon)} \,, \tag{2.68}$$

where the expression in the square brackets represents the microscopic occupation density. The other one is the *particle-number operator* $\hat{N}$, which is given as a continuous linear combination in terms of all occupation-density operators:

$$\hat{N} = \int d\alpha \, \hat{n}_\alpha = \int d\alpha \, \hat{b}_\alpha^\dagger \hat{b}_\alpha \, . \tag{2.69}$$

Because of (2.68), the basis states of $\mathcal{H}_N^{(\epsilon)}$ are also eigenstates of $\hat{N}$; here, the eigenvalue is always the total particle number N, so the eigenvalue equation reads

$$\hat{N} \, |\varphi_{1\alpha} \cdots \varphi_{N\alpha}\rangle^{(\epsilon)} = N \, |\varphi_{1\alpha} \cdots \varphi_{N\alpha}\rangle^{(\epsilon)} \, . \tag{2.70}$$

From the commutation relations for the creation and annihilation operators (2.61), (2.65), and (2.66), we obtain the commutators for both operators. For the occupation-density operator we get

$$\left[\hat{n}_\alpha, \hat{b}_\beta^\dagger\right]_- = \hat{b}_\alpha^\dagger \delta(\alpha - \beta) \, , \qquad \left[\hat{n}_\alpha, \hat{b}_\beta\right]_- = -\hat{b}_\alpha \delta(\alpha - \beta) \, , \tag{2.71}$$

and for the particle-number operator we have

$$\left[\hat{N}, \hat{b}_\alpha^\dagger\right]_- = \hat{b}_\alpha^\dagger \, , \qquad \left[\hat{N}, \hat{b}_\alpha\right]_- = -\hat{b}_\alpha \, . \tag{2.72}$$

At the beginning of this section, we made the assumption that the single-particle observable $\hat{\varphi}$, from whose eigenstates we constructed the basis of the N-particle Hilbert space $\mathcal{H}_N^{(\epsilon)}$, has a continuous spectrum. The prominent example of this type of observable is the *position operator* $\hat{\mathbf{x}}$. The corresponding creation and annihilation operators are the so-called *field operators* $\hat{\psi}^\dagger(\mathbf{x})$ and $\hat{\psi}(\mathbf{x})$, for which all of the relations found above hold naturally. Here, the special notation is as follows:

$$\hat{\psi}^\dagger(\mathbf{x}) \, |\mathbf{x}_1, \ldots, \mathbf{x}_N\rangle^{(\epsilon)} = \sqrt{N+1} \, |\mathbf{x}, \mathbf{x}_1, \ldots, \mathbf{x}_N\rangle^{(\epsilon)} \, , \tag{2.73}$$

$$|\mathbf{x}_1, \ldots, \mathbf{x}_N\rangle^{(\epsilon)} = \frac{1}{\sqrt{N!}} \, \hat{\psi}^\dagger(\mathbf{x}_1) \cdots \hat{\psi}^\dagger(\mathbf{x}_N) \, |0\rangle \, , \tag{2.74}$$

that is, the field operator $\hat{\psi}^\dagger(\mathbf{x})$ creates a particle at position $\mathbf{x}$. The commutation relations of the field operators follow immediately from (2.61), (2.65), and (2.66):

$$\begin{aligned} \left[\hat{\psi}^\dagger(\mathbf{x}), \hat{\psi}^\dagger(\mathbf{x}')\right]_{-\epsilon} &= \left[\hat{\psi}(\mathbf{x}), \hat{\psi}(\mathbf{x}')\right]_{-\epsilon} = 0 \, , \\ \left[\hat{\psi}(\mathbf{x}), \hat{\psi}^\dagger(\mathbf{x}')\right]_{-\epsilon} &= \delta(\mathbf{x} - \mathbf{x}') \, . \end{aligned} \tag{2.75}$$

We still have to find the relationship between the newly introduced field operators and the previous creation and annihilation operators (2.57) and (2.63). To this end, we use the single-particle completeness relation (2.40) for the position states $|\mathbf{x}\rangle$ with $|\varphi_\alpha\rangle$, obtaining

$$|\varphi_\alpha\rangle = \int d^D x \, |\mathbf{x}\rangle\langle\mathbf{x}\,|\,\varphi_\alpha\rangle = \int d^D x \, \varphi_\alpha(\mathbf{x}) |\mathbf{x}\rangle \, . \tag{2.76}$$

Thus, due to $|\varphi_\alpha\rangle = \hat{b}_\alpha^\dagger \, |0\rangle$ and $|\mathbf{x}\rangle = \hat{\psi}^\dagger(\hat{\mathbf{x}}) \, |0\rangle$, it follows that one can express the creation and annihilation operators in terms of the corresponding field operators as

$$\hat{b}_\alpha^\dagger = \int d^D x \, \varphi_\alpha(\mathbf{x}) \hat{\psi}^\dagger(\mathbf{x}) \, , \qquad \hat{b}_\alpha = \int d^D x \, \varphi_\alpha^*(\mathbf{x}) \hat{\psi}(\mathbf{x}) \, . \tag{2.77}$$

Here, it is important to note that $\varphi_\alpha(\mathbf{x})$ is the scalar wavefunction of the state $|\varphi_\alpha\rangle$, while $\hat{\psi}^\dagger(\mathbf{x})$ is an operator. The two relations in (2.77) can be reversed. With the completeness relation of the single-particle states $|\varphi_\alpha\rangle$ one obtains

$$\hat{\psi}^\dagger(\mathbf{x}) = \int d^D x \, \varphi_\alpha^*(\mathbf{x}) \hat{b}_\alpha^\dagger \, , \qquad \hat{\psi}(\mathbf{x}) = \int d^D x \, \varphi_\alpha(\mathbf{x}) \hat{b}_\alpha \, . \tag{2.78}$$

in analogy to (2.77). Finally, we may explicitly write down the (anti-)symmetrised many-particle states and the corresponding completeness relation in position representation, since we will refer to them later on in the main part of this thesis. Thus, in position representation, the (anti-)symmetrised many-particle states (2.42) read

$$|\mathbf{x}_{1a}, \ldots, \mathbf{x}_{Na}\rangle^{(\epsilon)} = \frac{1}{N!} \sum_P \epsilon^{p(P)} \, |\mathbf{x}_{P(1)a}, \ldots, \mathbf{x}_{P(N)a}\rangle \, , \tag{2.79}$$

and similarly, the completeness relation (2.55) is given by

$$\int d^D x_{1a} \cdots \int d^D x_{Na} \, |\mathbf{x}_{1a}, \ldots, \mathbf{x}_{Na}\rangle^{(\epsilon)} {}^{(\epsilon)}\langle \mathbf{x}_{1a}, \ldots, \mathbf{x}_{Na}| = \hat{\mathbb{1}} \, . \tag{2.80}$$

We now come to the notion of Fock space which is named after the Vladimir Aleksandrovich Fock and which is a suitable linear combination of the (anti-)symmetrised many-particle Hilbert spaces, thus allowing for arbitrary particle numbers N. More precisely, Fock space, denoted by $\mathcal{F}$, is the Hilbert space made from the infinite direct sum of (anti-)symmetrised N-particle Hilbert spaces $\mathcal{H}_N^{(\pm)}$ for all N:

$$\mathcal{F} \; = \; \mathcal{H}_1^{(\pm)} \; \oplus \; \mathcal{H}_2^{(\pm)} \; \oplus \; \mathcal{H}_3^{(\pm)} \; \oplus \; \cdots \; \oplus \; \mathcal{H}_n^{(\pm)} \; \oplus \; \cdots \tag{2.81}$$

It follows from the definition of $\mathcal{F}$ in (2.81) that the multi-particle Fock space position eigenstates living in $\mathcal{F}$ are of the form

$$|1; x_{1b}\rangle^{(\epsilon)} + |2; x_{1b}, x_{2b}\rangle^{(\epsilon)} + |3; x_{1b}, x_{2b}, x_{3b}\rangle^{(\epsilon)} + \cdots = \sum_{N=1}^{\infty} |N; x_{1b}, \ldots, x_{Nb}\rangle^{(\epsilon)} \; \in \mathcal{F} \, , \tag{2.82}$$

where an (anti-)symmetrised N-particle state (2.42) in (2.82) – which we have given an extra symbol N to distinguish states of different particle numbers – lives in the corresponding N-particle Hilbert space $\mathcal{H}_N^{(\pm)}$.

2.3.2 Discrete Fock Space of Occupation Number Eigenstates

We again assume the basis of the Hilbert space $\mathcal{H}_N^{(\epsilon)}$ of a system of N identical particles to be constructed from the eigenstates of the single-particle observable $\hat{\varphi}$. Whereas in the last section the single-particle observable $\hat{\varphi}$ was assumed to possess a continuous spectrum, in the present section we turn to the case of a discrete spectrum of $\hat{\varphi}$. The single-particle eigen equation (2.39) remains the same. The normalisation condition and the completeness relation now read:

$$\langle \varphi_\alpha \, | \, \varphi_\beta \rangle = \delta_{\alpha\beta} \, , \qquad \sum_\alpha |\varphi_\alpha\rangle\langle\varphi_\alpha| = \mathbb{1} \, . \tag{2.83}$$

Starting again with a non-symmetrised N-particle state of the form (2.41), and applying the symmetrisation operator (2.36), we obtain the (anti-)symmetrised N-particle state

$$|\varphi_{1\alpha}\cdots\varphi_{N\alpha}\rangle^{(\epsilon)} = C_\epsilon \sum_P \epsilon^{p(P)}\,\hat{P}(P)\,|\varphi_{1\alpha}\cdots\varphi_{N\alpha}\rangle = C_\epsilon \sum_P \epsilon^{p(P)}\,|\varphi_{P(1)\alpha}\cdots\varphi_{P(N)\alpha}\rangle \;, \tag{2.84}$$

which differs formally from (2.42) only by the normalisation constant. Thus, in the next step, we will determine the above normalisation constant C_ϵ. To this end, it is helpful to introduce the notion of occupation numbers n_i. These reflect the number of identical particles in the single particle state $|\varphi_{i\alpha}\rangle$. The sum of these must then yield the total particle number, i.e.

$$\sum_i n_i = N \;. \tag{2.85}$$

For bosons, where arbitrarily many particles can occupy the same quantum state, all values of n_i are allowed, i.e. $n_i = 1, 2, 3, \ldots$. On the contrary, for fermions, due to the Pauli principle, only the two values $n_i = 0, 1$ are permitted. Note, that we are not taking into account any spin degrees of freedom here. The constant C_ϵ is determined from the condition that the scalar product of the (anti-)symmetrised states (2.84) must be unity. Using (2.46)–(2.52) we obtain

$$1 = {}^{(\epsilon)}\langle\varphi_{1\alpha}\cdots\varphi_{N\alpha}\,|\,\varphi_{1\alpha}\cdots\varphi_{N\alpha}\rangle^{(\epsilon)} = \frac{C_\epsilon^2}{N!}\sum_P \epsilon^{p(P)}\,\langle\psi_{1\alpha}\,|\,\varphi_{P(1)\alpha}\rangle\langle\psi_{2\alpha}\,|\,\varphi_{P(2)\alpha}\rangle\cdots\langle\psi_{N\alpha}\,|\,\varphi_{P(N)\alpha}\rangle \;. \tag{2.86}$$

Here, because of the orthonormality (2.83) of the single-particle states, only those permutations contribute to the sum of (2.86) that have the effect of exchanging the particles in the n_i equivalent single-particle states $|\varphi_{i\alpha}\rangle$, where every one of these non-vanishing terms yields 1. Thus, all in all, there are

$$n_1!\,n_2!\,\cdots\,n_N! \tag{2.87}$$

such permutation and consequently, there are the same number of terms in the sum of (2.86). This leads to

$${}^{(\epsilon)}\langle\varphi_{1\alpha}\cdots\varphi_{N\alpha}\,|\,\varphi_{1\alpha}\cdots\varphi_{N\alpha}\rangle^{(\epsilon)} = \frac{C_\epsilon^2}{N!}\prod_{i=1}^{N} n_i! \;, \tag{2.88}$$

and finally, from (2.88) we can read off the normalisation constant. We have

$$C_+ = \frac{1}{\sqrt{N!\,\prod_{i=1}^{N} n_i!}} \qquad \text{for bosons,} \tag{2.89}$$

and, due to $0! = 1! = 1$,

$$C_- = \frac{1}{\sqrt{N!}} \qquad \text{for fermions.} \tag{2.90}$$

We see, that the (anti-)symmetrised many-particle state $|\varphi_{1\alpha}\cdots\varphi_{N\alpha}\rangle^{(\epsilon)}$ is uniquely defined by specifying the infinitely many occupation numbers $n_1, n_2, \ldots$. This leads to the so-called *occupation-number representation*, or discrete Fock space representation:

$$|N; n_1, n_2, \ldots, n_i, \ldots\rangle^{(\epsilon)} \equiv |\varphi_{1\alpha}\cdots\varphi_{N\alpha}\rangle^{(\epsilon)} \;, \tag{2.91}$$

where in the symbol for the state, i.e. for the ket, *all* occupation numbers are given and where the unoccupied single-particle states are denoted by $n_i = 0$. It is clear that two such states are identical if and only if they have the same occupation numbers, thus from the single-particle states we obtain the following orthonormalisation relation:

$$^{(\epsilon)}\langle N; \ldots, n_i, \ldots | N'; \ldots, n'_i, \ldots \rangle^{(\epsilon)} = \delta_{N,N'} \prod_i \delta_{n_i, n'_i} \ . \tag{2.92}$$

Equally, we have the completeness relation

$$\sum_{n_1} \sum_{n_2} \cdots \sum_{n_i} \cdots | N; \ldots, n_i, \ldots \rangle^{(\epsilon)(\epsilon)} \langle N'; \ldots, n'_i, \ldots | = \mathbb{1} \ . \tag{2.93}$$

The sum in (2.93) runs over all occupation numbers that satisfy the condition $\sum_i n_i = N$.

In occupation-number representation, the definition of creation and annihilation operators is straightforward, however, due to the different normalisation constants (2.89) and (2.89), we must now explicitly distinguish between bosonic and fermionic ones. For bosons, the creation operator is defined by its action on a state in occupation-number representation:

$$\hat{b}_i^\dagger \, | N; \ldots, n_i, \ldots \rangle^{(+)} = \sqrt{n_i + 1} \, | N+1; \ldots, n_i + 1, \ldots \rangle^{(+)} \ ; \tag{2.94}$$

and similarly, for fermions we have

$$\hat{a}_i^\dagger \, | N; \ldots, n_i, \ldots \rangle^{(-)} = (-1)^{N_i} \, \delta_{n_i,0} \, | N+1; \ldots, n_i + 1, \ldots \rangle^{(-)} \ . \tag{2.95}$$

As in the case of the continuous Fock space, every N-particle state in the discrete Fock space can be created from the vacuum state by repeated application of the creation operator:

$$| N; n_1, n_2, \ldots, n_i, \ldots \rangle^{(\epsilon)} = \prod_{p=1}^{\sum n_p = N} \frac{(\hat{b}_p^\dagger)^{n_p}}{\sqrt{n_p!}} \, \epsilon^{N_p} \, | 0 \rangle \ . \tag{2.96}$$

The annihilation operator is again defined as the adjoint of the creation operator. Its action is given by

$$\hat{b}_i \, | N; \ldots, n_i, \ldots \rangle^{(+)} = \sqrt{n_i} \, | N-1; \ldots, n_i - 1, \ldots \rangle^{(+)} \ ; \tag{2.97}$$

for the bosonic case and by

$$\hat{a}_i \, | N; \ldots, n_i, \ldots \rangle^{(-)} = (-1)^{N_i} \, \delta_{n_i,1} \, | N-1; \ldots, n_i - 1, \ldots \rangle^{(-)} \ . \tag{2.98}$$

for fermions, where the limitations on the particle number are taken into account by the extra factor $\delta_{n_i,1}$. The fundamental commutation relations for the bosonic and fermionic creation and annihilation operators can be found by calculating the action of two of these on occupation number states (2.91), for example, we have

$$\begin{aligned} \hat{b}_i^\dagger \, \hat{b}_j^\dagger \, | \ldots, n_i, \ldots, n_j, \ldots \rangle^{(+)} &= \sqrt{n_i + 1} \sqrt{n_j + 1} \, | \ldots, n_i + 1, \ldots, n_j + 1, \ldots \rangle^{(+)} \\ &= \hat{b}_j^\dagger \, \hat{b}_i^\dagger \, | \ldots, n_i, \ldots, n_j, \ldots \rangle^{(+)} \ , \end{aligned} \tag{2.99}$$

for products of bosonic creation operators, and

$$\begin{aligned} \hat{b}_i^\dagger \, \hat{b}_j \, | \ldots, n_i, \ldots, n_j, \ldots \rangle^{(+)} &= \sqrt{n_j} \sqrt{n_i + 1} \, | \ldots, n_i + 1, \ldots, n_j - 1, \ldots \rangle^{(+)} \\ &= \hat{b}_j \, \hat{b}_i^\dagger \, | \ldots, n_i, \ldots, n_j, \ldots \rangle^{(+)} \end{aligned} \tag{2.100}$$

for products of bosonic creation and annihilation operators. The derivation of the other combinations for bosons and for fermions is straightforward and can be found, e.g., in [24]. They yield the following commutation relations:

$$\left[\hat{b}_i^\dagger, \hat{b}_j^\dagger\right]_{-\epsilon} = \left[\hat{b}_i, \hat{b}_j\right]_{-\epsilon} = 0 \;, \qquad \left[\hat{b}_i, \hat{b}_j^\dagger\right]_{-\epsilon} = \delta_{ij} \;, \tag{2.101}$$

for bosons, and equally:

$$\left[\hat{a}_i^\dagger, \hat{a}_j^\dagger\right]_{-\epsilon} = \left[\hat{a}_i, \hat{a}_j\right]_{-\epsilon} = 0 \;, \qquad \left[\hat{a}_i, \hat{a}_j^\dagger\right]_{-\epsilon} = \delta_{ij} \;, \tag{2.102}$$

for fermions. In analogy to the the occupation density operator (2.67), we have in the discrete case of the occupation number representation the *occupation-number operator*

$$\hat{n}_i^{(+)} = \hat{b}_i^\dagger \hat{b}_i \;, \qquad \hat{n}_i^{(-)} = \hat{a}_i^\dagger \hat{a}_i \;, \tag{2.103}$$

for bosons and fermions, respectively. When dealing with general occupation-number operators, we will drop the superscript $(+)$ and $(-)$ from now on. From (2.100) we see, that the occupation-number states are eigenstates of $\hat{n}_i$, as the name already implies:

$$\hat{n}_i \left|N; \ldots, n_i, \ldots\right\rangle^{(\epsilon)} = n_i \left|N; \ldots, n_i, \ldots\right\rangle^{(\epsilon)} \;. \tag{2.104}$$

Here, the eigenvalue n_i is, of course, the occupation-number of the ith single-particle state in (2.104). The particle number operator in occupation-number representation reads in analogy to (2.69):

$$\hat{N} = \sum_i \hat{n}_i \;. \tag{2.105}$$

As (2.105) is constructed from a sum of occupation-number operators, it satisfies the same eigenvalue equation,

$$\hat{N} \left|N; \ldots, n_i, \ldots\right\rangle^{(\epsilon)} = N \left|N; \ldots, n_i, \ldots\right\rangle^{(\epsilon)} \;, \tag{2.106}$$

where the eigenvalue is the total particle number N.

Chapter 3

Ideal Quantum Gases in Canonical and Grand-Canonical Ensembles

3.1 Statistical Mechanics

Statistical mechanics is the underlying microscopical theory of thermodynamics. As such it provides a framework for relating the microscopic properties of the constituent particles, i.e. atoms or molecules of a given system to its macroscopic or bulk properties. Mathematically, it results from the application of probability theory to the field of mechanics where the N-particle system in question is treated as a statistical ensemble, i.e. as the set of all possible microstates of the system that share the same macrostate. The statistical properties of the ensemble then depend on a chosen probability measure on the phase space, the choice of which is dictated by the specific details of the system and the assumptions one makes about the ensemble in general. The correct probability measure or distribution function ρ for a system is that one which maximises its entropy; this is in accordance with the second law of thermodynamics, which states that the entropy, i.e. the amount of disorder, of a closed system can only increase. The entropy is defined as

$$S = -k_{\mathrm{B}} \sum_{i} \rho_i \ln \rho_i \ , \tag{3.1}$$

where k_{B} is the Boltzmann constant. The sum runs over all microstates which are consistent with the given macrostate and ρ_i is proportional to the probability of the ith microstate. As ρ_i is a probability measure, it is normalized to unity and the normalising factor of ρ_i is referred to as the partition function of the ensemble. This is a quantity that encodes the statistical properties of a system in thermodynamic equilibrium and its importance lies in the fact that all thermodynamic quantities of the system can be calculated from it.

3.1.1 Microcanonical Ensemble

The most basic ensemble of statistical mechanics is the so-called microcanonical ensemble, where the possible states of the system all have the same energy and the probability for the system to be in any given state is the same. Thus, all systems of the ensemble have the same number of particles N, the same volume V and the same energy U, so a microcanonical ensemble describes an isolated system. If Ω is the number of accessible microstates, the probability that a system chosen at random from the ensemble would be in a given microstate is $1/\Omega$. From Ω we then obtain the entropy of the system via

$$S = k_{\mathrm{B}} \ln \Omega \ , \qquad \text{or equivalently} \qquad \Omega(U, V, N) = \mathrm{e}^{S/k_{\mathrm{B}}} \ . \tag{3.2}$$

In the microcanonical ensemble, Ω assumes the role of the partition function, as well as that of the characteristic state function.

3.1.2 Canonical Ensemble

If we couple a system to a heat bath, i.e. to an infinitely large reservoir of thermal energy, the energy of the system can fluctuate around its mean value, which in turn is fixed by the heat bath. This type of system, where volume V and particle number N are constant is described by the canonical ensemble. Extremalisation of the entropy under the above conditions leads to the Boltzmann distribution and thus to the following distribution function:

$$\rho_i = \frac{1}{Z(\beta)}\,\mathrm{e}^{-\beta E_i}\ . \tag{3.3}$$

Here, $\beta = 1/(k_\mathrm{B}T)$ is the inverse temperature. The quantum mechanical version of the distribution function is the canonical density operator

$$\hat{\varrho} = \frac{1}{Z(\beta)}\,\mathrm{e}^{-\beta \hat{H}}\ , \tag{3.4}$$

where $\hat{H}$ is the Hamiltonian that governs the time-evolution of the system. It describes the mixed state of a canonical ensemble of quantum mechanical systems. The partition function is then given by the trace of the operator-valued Boltzmann factor in (3.4):

$$Z(\beta) = \mathrm{Tr}\left\{\mathrm{e}^{-\beta\hat{H}}\right\}\ . \tag{3.5}$$

If we carry out the trace in the eigenbasis of the Hamiltonian, which we assume to be discrete without loss of generality, we obtain

$$Z(\beta) = \sum_i \langle n|\,\mathrm{e}^{-\beta\hat{H}}\,|n\rangle = \sum_i \mathrm{e}^{-\beta E_i}\ , \tag{3.6}$$

where the exponential is called a Boltzmann weight and E_i is the energy of the ith eigenstate. For a continuous eigenbasis the trace in (3.5) is also continuous, i.e. the sum in the first equation of (3.6) must be replaced by an integral.

Let $\hat{A}$ be a physical observable, then its thermal expectation value is given by the trace with the density operator, i.e.

$$\langle\hat{A}\rangle = \mathrm{Tr}\,\{\hat{\varrho}\,\hat{A}\}\ . \tag{3.7}$$

The characteristic state function of the canonical ensemble is the Helmholtz free energy, or free energy for short:

$$F = -\frac{1}{\beta}\ln Z(\beta)\ , \tag{3.8}$$

which assumes a minimum in thermodynamic equilibrium.

3.1.3 Grand-Canonical Ensemble

The grand-canonical ensemble is a generalisation of the canonical ensemble, in that the system is additionally coupled to a particle reservoir. It describes an open system which can exchange thermal energy and particles with its environment. Thus a system, where only the volume V is constant, and both the internal energy U and the particle number N are allowed to fluctuate, is described by the grand-canonical ensemble. Under these conditions, the extremalization of the entropy results in the grand-canonical distribution function

$$\rho_i = \frac{1}{\mathcal{Z}(\beta)} \, \mathrm{e}^{-\beta(E_i - \mu N_i)} \; . \tag{3.9}$$

A mixed state of a grand-canonical ensemble of quantum systems is then described by the grand-canonical density operator

$$\hat{\varrho}_{\mathrm{GK}} = \frac{1}{\mathcal{Z}(\beta)} \, \mathrm{e}^{-\beta(\hat{H} - \mu \hat{N})} \; , \tag{3.10}$$

Here, μ is the chemical potential, which is a measure for the energy associated with the exchange of a single particle, $\hat{N}$ represents the particle number operator, and $\mathcal{Z}(\beta)$ denotes the grand-canonical partition function

$$Z(\beta) = \mathrm{Tr}\left\{\hat{\varrho}_{\mathrm{GK}}\right\} = \mathrm{Tr}\left\{\mathrm{e}^{-\beta(\hat{H} - \mu \hat{N})}\right\} \; . \tag{3.11}$$

In a basis, where the Hamiltonian is diagonal,the latter reads

$$\mathcal{Z}(\beta) = \sum_i \mathrm{e}^{-\beta(E_i - \mu N_i)} \; , \tag{3.12}$$

where N_i is the particle number in the ith eigenstate of $\hat{H}$. As in the canonical ensemble in (3.7), the grand-canonical thermal expectation value of an observable $\hat{A}$ is given by the trace of $\hat{A}$ with the grand-canonical density operator (3.10):

$$\langle \hat{A} \rangle = \mathrm{Tr}\left\{\hat{\varrho}_{\mathrm{GK}} \, \hat{A}\right\} \; . \tag{3.13}$$

The characteristic state function of the grand canonical ensemble is the grand canonical free energy

$$\mathcal{F} = -\frac{1}{\beta} \ln \mathcal{Z}(\beta) \; . \tag{3.14}$$

Note, that throughout this thesis, we use calligraphic letters for grand-canonical quantities, e.g. $\mathcal{Z}$ for the grand-canonical partition function and $\mathcal{F}$ for the grand-canonical free energy, which is often called the grand potential.

3.2 One-Particle Time Evolution Amplitude

The most important quantity in the path-integral formulation of quantum statistics is the quantum mechanical time evolution amplitude

$$(\mathbf{x}_b, t_b | \mathbf{x}_a, t_a) = \langle \mathbf{x}_b | \, \mathrm{e}^{-i\hat{H}(t_b - t_a)/\hbar} \, | \mathbf{x}_a \rangle \; , \tag{3.15}$$

which we obtain by sandwiching the time evolution operator of the system of interest between suitable basis states, e.g. between position eigenstates $\langle \mathbf{x}_b|$ and $|\mathbf{x}_a\rangle$.

Now, comparing the Boltzmann factor $\exp\{-\beta\hat{H}\}$ of the canonical ensemble to the quantum mechanical time evolution operator $\exp\{-i\hat{H}(t_b - t_a)/\hbar\}$, we observe that they have a similar form, both containing the Hamiltonian $\hat{H}$, and we obtain the former by an analytic continuation of $\exp\{-i\hat{H}(t_b - t_a)/\hbar\}$ via

$$t_b - t_a = -i\hbar\beta \tag{3.16}$$

to imaginary time. This procedure is called Wick rotation after the Italian physicist Gian-Carlo Wick. Thus, Wick rotation connects the equilibrium thermodynamics of statistical mechanics to the quantum mechanical time evolution of a system by replacing inverse temperature β with imaginary time $it/\hbar$. It is an invaluable tool that is widely used throughout the field of theoretical physics as it allows one to use the formalism and the methods of statistical physics for solving quantum mechanical problems and vice versa.

Performing a Wick rotation on the quantum mechanical real-time evolution amplitude (3.15), we obtain the so-called imaginary-time evolution amplitude

$$(\mathbf{x}_b, \tau_b|\mathbf{x}_a, \tau_a) = \langle \mathbf{x}_b|\, \mathrm{e}^{-\beta\hat{H}}\, |\mathbf{x}_a\rangle = (\mathbf{x}_b, t_b|\mathbf{x}_a, t_a)\Bigg|_{t_a=0}^{t_b=\hbar\beta} \,, \tag{3.17}$$

According to (3.5), its trace yields the partition function

$$Z(\beta) = \int d^D x\, (\mathbf{x}, \hbar\beta|\mathbf{x}, 0) \,, \tag{3.18}$$

and from (3.4) we see that the density matrix is given by the normalized amplitude (3.17),

$$\varrho(\mathbf{x}_b, \mathbf{x}_a) = \frac{1}{Z(\beta)}\, (\mathbf{x}_b, \hbar\beta|\mathbf{x}_a, 0) \,. \tag{3.19}$$

The imaginary-time evolution amplitude (3.17) has the following properties, which it inherits from its real-time counterpart (3.15):

- Invariance under time translations:

$$(\mathbf{x}_b, \tau_b + \tau_0|\mathbf{x}_a, \tau_a + \tau_0) = (\mathbf{x}_b, \tau_b|\mathbf{x}_a, \tau_a) \,. \tag{3.20}$$

- Invariance under time reversal:

$$(\mathbf{x}_a, \tau_a|\mathbf{x}_b, \tau_b) = (\mathbf{x}_b, \tau_b|\mathbf{x}_a, \tau_a)^* \,. \tag{3.21}$$

- It obeys the Schrödinger equation:

$$i\hbar\frac{\partial}{\partial\tau_b}\, (\mathbf{x}_b, \tau_b|\mathbf{x}_a, \tau_a) = \langle \mathbf{x}_b|\, \hat{H}\, \mathrm{e}^{-\hat{H}(\tau_b-\tau_a)}\, |\mathbf{x}_a\rangle = \hat{H}(\mathbf{x}_b)\, (\mathbf{x}_b, \tau_b|\mathbf{x}_a, \tau_a) \,, \tag{3.22}$$

where $\tau_b = it_b/\hbar$ and $\tau_a = it_a/\hbar$.

- It solves the initial value problem of the Schrödiger equation (3.22) for ψ_0,
  $$\psi(\mathbf{x}_b, \tau_b) = \int d^D x_a \, (\mathbf{x}_b, \tau_b | \mathbf{x}_a, \tau_a) \, \psi_0(\mathbf{x}_a, \tau_a) \, , \tag{3.23}$$
  as it is also the propagator, i.e. the Greens function of the Hamiltonian $\hat{H}$.
- Spectral representation:
  $$(\mathbf{x}_b, \tau_b | \mathbf{x}_a, \tau_a) = \sum_n \langle \mathbf{x}_b \, | \, n \rangle \, \langle n \, | \, \mathbf{x}_a \rangle \, \mathrm{e}^{-E_n(\tau_b - \tau_a)} = \sum_n \psi_n \, (\mathbf{x}_b) \psi_n^*(\mathbf{x}_a) \, \mathrm{e}^{-E_n(\tau_b - \tau_a)} \, , \tag{3.24}$$
  where $\psi_n(\mathbf{x}) = \langle \mathbf{x}_b \mid n \rangle$ are the position eigenfunctions of the Hamiltonian, satisfying $\hat{H}(\mathbf{x})\psi_n(\mathbf{x}) = E_n \psi_n(\mathbf{x})$. We obtain (3.24) by inserting into (3.17) the completeness relation of the eigenstates $|n\rangle$.
- Group property:
  $$(\mathbf{x}_b, \tau_b | \mathbf{x}_a, \tau_a) = \int d^D x_c \, (\mathbf{x}_b, \tau_b | \mathbf{x}_c, \tau_c) \, (\mathbf{x}_c, \tau_c | \mathbf{x}_a, \tau_a) \tag{3.25}$$
  This is a consequence of the group property of the time evolution operator. It follows from (3.15) by splitting the time evolution operator into two pieces at some arbitrary intermediate time t_c and inserting the completenes relation of the states $|\mathbf{x}_c\rangle$ in between, prior to Wick rotating it to imaginary time.

The last property is the most important one, as it enables us to derive a path integral for the imaginary-time evolution amplitude (3.17).

3.3 Path Integral

The path integral formulation of quantum mechanics, due to Feynman, exploits the group property (3.25) of the time evolution operator, where the Hamiltonian in its exponent is the infinitesimal generator of time-translations, together with the superposition principle. The amplitude for a quantum mechanical particle to go from one point in space to another is given by (3.15). Because of said group property, the time evolution operator can be split into a product of $N + 1$ time evolution operators, each one acting only during a short time step

$$\Delta t = \frac{t_b - t_a}{N + 1} \, , \tag{3.26}$$

so we have

$$(\mathbf{x}_b, t_b | \mathbf{x}_a, t_a) = \langle \mathbf{x}_b | \underbrace{\mathrm{e}^{-i\hat{H}\Delta t/\hbar} \, \mathrm{e}^{-i\hat{H}\Delta t/\hbar} \cdots \mathrm{e}^{-i\hat{H}\Delta t/\hbar}}_{N \text{ factors}} | \mathbf{x}_a \rangle \, . \tag{3.27}$$

Between these, we may insert N completeness relations, each contributing an integral over the intermediate states, yielding N D-dimensional integrals of a product of N time-evolution amplitudes:

$$(\mathbf{x}_b, t_b | \mathbf{x}_a, t_a) = \int_{-\infty}^{\infty} d^D x_N \cdots \int_{-\infty}^{\infty} d^D x_1 \, \langle \mathbf{x}_b | \, \mathrm{e}^{-i\hat{H}\Delta t/\hbar} \, | \mathbf{x}_N \rangle \, \langle \mathbf{x}_N | \, \mathrm{e}^{-i\hat{H}\Delta t/\hbar} \, | \mathbf{x}_{N-1} \rangle \cdots$$
$$\cdots \langle \mathbf{x}_1 | \, \mathrm{e}^{-i\hat{H}\Delta t/\hbar} \, | \mathbf{x}_a \rangle \, . \tag{3.28}$$

Writing this in a more compact way, we have

$$(\mathbf{x}_b, t_b|\mathbf{x}_a, t_a) = \left\{ \prod_{n=1}^{N} \int_{-\infty}^{\infty} d^D x_n \right\} \prod_{n=1}^{N+1} (\mathbf{x}_n, \Delta t|\mathbf{x}_{n-1}, 0) \ , \tag{3.29}$$

where

$$(\mathbf{x}_n, \Delta t|\mathbf{x}_{n-1}, 0) = \langle \mathbf{x}_n | \, \mathrm{e}^{-i\hat{H}\Delta t/\hbar} \, |\mathbf{x}_{n-1}\rangle \tag{3.30}$$

is referred to as a short-time amplitude, and where we have made the identifications $\mathbf{x}_0 = \mathbf{x}_a$ and $\mathbf{x}_{N+1} = \mathbf{x}_b$. If we assume the Hamiltonian in (3.30) to be of the standard form $\hat{H} = \hat{T}(\hat{\mathbf{p}}) + \hat{V}(\hat{\mathbf{x}})$, where $\hat{T}$ and $\hat{V}$ are the kinetic and potential energy, respectively, we may use the Baker-Campbell-Hausdorff formula (see [22, appendix 2A]) to write the short-time amplitude explicitly as

$$(\mathbf{x}_n, \Delta t|\mathbf{x}_{n-1}, 0) = \langle \mathbf{x}_n | \, \mathrm{e}^{-i\hat{\mathbf{p}}^2\Delta t/2M\hbar} \, \mathrm{e}^{-i\hat{V}(\hat{\mathbf{x}})\Delta t/\hbar} \mathrm{e}^{-i\hat{O}\Delta t/\hbar} \, |\mathbf{x}_{n-1}\rangle \ . \tag{3.31}$$

The operator $\hat{O}$, that appears in the last exponential of (3.31), is of order $\mathcal{O}((\Delta t)^2)$ and contains nested commutators of $\hat{p}$ and $\hat{V}$. It will tend to zero, when we take the limit $\Delta t \to 0$ later on, so we will neglect it from now on. We can swap the squared momentum operator in the short time amplitude above with its eigenvalue squared by inserting the D-dimensional completeness relation for momentum eigenstates after the first exponential operator in (3.31). Similarly, we may let the potential energy operator $\hat{V}(\hat{\mathbf{x}})$ act on the position eigenstate to the right. Here we note, that up to first order in Δt it holds that $V(\mathbf{x}_{n-1}) = V(\mathbf{x}_n)$, so $V(\mathbf{x}_{n-1})$ will tend to $V(\mathbf{x}_n)$ in the above limit, and we can write

$$(\mathbf{x}_n, \Delta t|\mathbf{x}_{n-1}, 0) \approx \int_{-\infty}^{\infty} d^D p_n \, \langle \mathbf{x}_n \,|\, \mathbf{p}_n\rangle \, \langle \mathbf{p}_n \,|\, \mathbf{x}_{n-1}\rangle \, \mathrm{e}^{-i\mathbf{p}_n^2\Delta t/2M\hbar} \, \mathrm{e}^{-iV(\mathbf{x}_n)\Delta t/\hbar} \ . \tag{3.32}$$

Using the fact that the momentum eigenstates in terms of $\mathbf{x}$, i.e., $\psi_{\mathbf{p}}(\mathbf{x}) = \langle \mathbf{x} \,|\, \mathbf{p}\rangle$, are plane waves, i.e.

$$\psi_{\mathbf{p}}(\mathbf{x}) = \frac{\mathrm{e}^{i\mathbf{p}\mathbf{x}/\hbar}}{(2\pi\hbar)^{D/2}} \ , \tag{3.33}$$

equation (3.32) becomes a Fresnel integral,

$$(\mathbf{x}_n, \Delta t|\mathbf{x}_{n-1}, 0) \approx \int_{-\infty}^{\infty} \frac{d^D p_n}{(2\pi\hbar)^D} \, \mathrm{e}^{-i\mathbf{p}_n^2\Delta t/2M\hbar} \, \mathrm{e}^{-iV(\mathbf{x}_n)\Delta t/\hbar} \, \mathrm{e}^{i\mathbf{p}_n(\mathbf{x}_n-\mathbf{x}_{n-1})/\hbar} \ . \tag{3.34}$$

Writing the three exponentials in (3.34) as a single one, and recalling from classical mechanics the form of the inverse Legendre transformation

$$\mathcal{L}(\mathbf{x}, \dot{\mathbf{x}}) = \mathbf{p} \cdot \dot{\mathbf{x}} - H(\mathbf{x}, \mathbf{p}) \ , \tag{3.35}$$

we find the combined exponent to be i times the discretised classical Lagrangian at timestep t_n, times Δt, which is equal to the discretised action at step n:

$$\frac{i}{\hbar}\left[\mathbf{p}_n \cdot \Big(\frac{\mathbf{x}_n - \mathbf{x}_{n-1}}{\Delta t}\Big) - \Big(\frac{\mathbf{p}_n^2}{2M} + V(\mathbf{x}_n)\Big)\right]\Delta t = \frac{i}{\hbar}\Big[\mathbf{p}_n(t_n) \cdot \dot{\mathbf{x}}_n(t_n) - H(\mathbf{p}_n, \mathbf{x}_n)\Big]\Delta t \ , \tag{3.36}$$

that is

$$\mathcal{A}_n(\mathbf{x}_n, \dot{\mathbf{x}}_n) = \mathcal{L}(\mathbf{x}_n, \dot{\mathbf{x}}_n)\, \Delta t\,. \tag{3.37}$$

When we insert this into (3.29), we obtain the expression for the time evolution amplitude as a discretised path integral in phase space

$$(\mathbf{x}_b, t_b|\mathbf{x}_a, t_a) = \lim_{\Delta t \to 0} \left\{ \prod_{n=1}^{N} \int_{-\infty}^{\infty} d^D x_n \right\} \left\{ \prod_{n=1}^{N+1} \int_{-\infty}^{\infty} \frac{d^D p_n}{(2\pi\hbar)^D} \right\} \mathrm{e}^{i\mathcal{A}^{(N)}/\hbar}\,, \tag{3.38}$$

where

$$\mathcal{A}^{(N)} = \sum_{n=1}^{N+1} \left\{ \mathbf{p}_n \cdot \left[\frac{\mathbf{x}_n - \mathbf{x}_{n-1}}{\Delta t} \right] - \left[\frac{\mathbf{p}_n^2}{2M} + V(\mathbf{x}_n) \right] \right\} \Delta t \tag{3.39}$$

is the discretised action. In the limit of $N \to \infty$, corresponding to infinitesimal timesteps $\Delta t \to dt$, the sum in (3.39) tends to an integral, yielding the classical action in phase space

$$\mathcal{A}^{(N)}[\mathbf{x}, \mathbf{p}] = \int_{t_a}^{t_b} dt\, \left\{ \mathbf{p}(t) \cdot \dot{\mathbf{x}}(t) - \left[\frac{\mathbf{p}^2(t)}{2M} + V(\mathbf{x}(t)) \right] \right\}\,, \tag{3.40}$$

and (3.38) becomes the phase space path integral

$$(\mathbf{x}_b, t_b|\mathbf{x}_a, t_a) = \int_{\mathbf{x}(t_a)=\mathbf{x}_a}^{\mathbf{x}(t_b)=\mathbf{x}_b} \frac{\mathcal{D}'\mathbf{x}\mathcal{D}\mathbf{p}}{(2\pi\hbar)^D}\, \mathrm{e}^{i\mathcal{A}[\mathbf{x},\mathbf{p}]/\hbar}\,. \tag{3.41}$$

Here the calligraphic capital $\mathcal{D}$ stands for the infinite product of integrals in (3.38) and the prime indicates that in the configuration space measure of (3.38) there is one D dimensional integral less than in the momentum space measure.

Thus the time evolution amplitude is given by a continuous superposition, i.e. a contiuous sum over all paths connecting the initial and final points $\mathbf{x}_a$ and $\mathbf{x}_b$, where the contribution of each path is weighed by the classical action along the trajectory. In the path integral picture of quantum mechanics a particle moves along all possible paths simultaneously; however, for those paths which do not extremalise the action (3.40), the phase factor in (3.41) oscillates wildly, leading to destructive interference of the path with itself in accordance with the Riemann-Lebesgue lemma.

If instead, we solve the Fresnel integral in (3.34), i.e.

$$(\mathbf{x}_n, \Delta t|\mathbf{x}_{n-1}, 0) \approx \left(\frac{M}{2\pi i\hbar\Delta t} \right)^{D/2} \exp\left\{ \frac{iM(\mathbf{x}_n - \mathbf{x}_{n-1})^2}{2\hbar\Delta t} - \frac{i}{\hbar} V(\mathbf{x}_n)\Delta t \right\}\,, \tag{3.42}$$

and insert this into (3.29), we obtain the time-sliced path integral in configuration space

$$(\mathbf{x}_b, t_b|\mathbf{x}_a, t_a) = \lim_{\Delta t \to 0} \left\{ \prod_{n=1}^{N} \int_{-\infty}^{\infty} d^D x_n \right\} \left(\frac{M}{2\pi i\hbar\Delta t} \right)^{D(N+1)/2} \mathrm{e}^{i\mathcal{A}^{(N)}/\hbar}\,, \tag{3.43}$$

where $\mathcal{A}^{(N)}$ is the time-sliced action

$$\mathcal{A}^{(N)} = \sum_{n=1}^{N+1} \left\{ \frac{M}{2} \left[\frac{\mathbf{x}_n - \mathbf{x}_{n-1}}{\Delta t} \right]^2 - V(\mathbf{x}_n) \right\} \Delta t\,. \tag{3.44}$$

Note that, when in (3.43) we take the limit $N \to \infty$, $\Delta t \to dt$, there appears a diverging factor of $1/(\Delta t)^{D(N+1)/2}$, which is removed only after doing the N D-dimensional x-integrals. Thus, we obtain the path integral in configuration space,

$$(\mathbf{x}_b, t_b|\mathbf{x}_a, t_a) = \int_{\mathbf{x}(t_a)=\mathbf{x}_a}^{\mathbf{x}(t_b)=\mathbf{x}_b} \mathcal{D}\mathbf{x}\, \mathrm{e}^{i\mathcal{A}[\mathbf{x}]/\hbar} \ . \tag{3.45}$$

From the definition of the Wick rotation (3.16) we see that the imaginary-time evolution amplitude (3.17) may equally be calculated from the following path integral:

$$(\mathbf{x}_b, \hbar\beta|\mathbf{x}_a, 0) = \int_{\mathbf{x}(0)=\mathbf{x}_a}^{\mathbf{x}(\hbar\beta)=\mathbf{x}_b} \mathcal{D}\mathbf{x}\, \mathrm{e}^{-i\mathcal{A}[\mathbf{x}]/\hbar} \ . \tag{3.46}$$

Here, the action in the exponential of (3.46) is the Euclidean action

$$\mathcal{A}[\mathbf{x}] = \int_0^{\hbar\beta} d\tau \left\{ \frac{M}{2}\dot{\mathbf{x}}^2(\tau) + V(\mathbf{x}(\tau)) \right\} \ . \tag{3.47}$$

3.4 Ideal Quantum Gases in Canonical Ensemble

This section lays the foundations for the canonical description of ideal quantum gases. We begin by introducing the so-called Van-Vleck-Pauli-Morette formula for the time-evolution amplitude, with which we then calculate the time evolution amplitude of the harmonic oscillator. Finally, we derive the canonical partition function, both in cycle-reduced form and in the form of a recursion.

3.4.1 Van-Vleck-Pauli-Morette Formula

In the following, we sketch briefly what is called the semiclassical expansion within the path integral formalism [22, Chapter 4.2]; a method that was pioneered by DeWitt-Morette in the early 1950s [25]. In the end we obtain the general Van-Vleck-Pauli-Morette formula, which we will use to derive the expression for the time evolution amplitude of the harmonic oscillator in the next subsection.

This is done by applying the saddle point expansion to the configuration space path integral (3.45). According to the last section, the contribution of each path to the amplitude (3.15) is given by an exponential of the ratio of the classical action along the path to the reduced Planck constant $\hbar$. As long as typical fluctuations of the action are much larger than $\hbar$, i.e. for paths that deviate significantly from the classical one, the exponential in (3.45) oscillates strongly, and the amplitudes of these paths effectively cancel each other by interference. Thus, the dominant contribution to (3.45) comes from the functional regime where oscillations are weakest, i.e. from the extremum of the action where

$$\frac{\delta\mathcal{A}[x]}{\delta x(t)} = 0 \ . \tag{3.48}$$

Consequently, we see that the behaviour of the time evolution amplitude is given by the saddle point expansion of the path integral around the classical path where (3.48) holds. In other words we expand the exponent of (3.45), that is the classical action

$$\mathcal{A}[x,\dot{x}] = \int_{t_a}^{t_b} dt\, \left[\frac{M}{2}\dot{x}^2 - V(x)\right] , \tag{3.49}$$

around the classical particle orbit in powers of the fluctuations $\delta x = x(t) - x_{\rm cl}(t)$, i.e. of the deviations from the classical path. This is known as a fluctuation expansion:

$$\mathcal{A}[x,\dot{x}] = \mathcal{A}[x_{\rm cl}] + \int_{t_a}^{t_b} dt\, \frac{\delta \mathcal{A}}{\delta x(t)}\bigg|_{x(t)=x_{\rm cl}(t)} \delta x(t) + \frac{1}{2}\int_{t_a}^{t_b} dt\, dt'\, \frac{\delta^2 \mathcal{A}}{\delta x(t), \delta x(t')}\bigg|_{x(t)=x_{\rm cl}(t)} \delta x(t)\, \delta x(t') + \ldots\ . \tag{3.50}$$

In this *fluctuation expansion* the linear term is zero because of the condition (3.48). If we carry out the above expansion up to quadratic order, we are left with an exponential of the classical action $\mathcal{A}[x_{\rm cl}]$, times the path integral over an exponential of the quadratic fluctuations of the action. Thus we find that the leading term in the semiclassical approximation to the time evolution amplitude is given by

$$(x_b, t_b | x_a, t_a)_{\rm sc} = F(x_b, t_b; x_a, t_a)\, {\rm e}^{i\mathcal{A}(x_b,t_b;x_a,t_a)/\hbar} , \tag{3.51}$$

where $F(x_b, t_b; x_a, t_a)$ is called a fluctuation factor. For a point particle, the quadratic term is

$$\frac{1}{2}\int_{t_a}^{t_b} dt\, dt'\, \frac{\delta^2 \mathcal{A}}{\delta x(t)\, \delta x(t')}\bigg|_{x(t)=x_{\rm cl}(t)} \delta x(t)\, \delta x(t') = \int_{t_a}^{t_b} dt\, \left[\frac{M}{2}(\delta\dot{x})^2 + \frac{1}{2}V''(x_{\rm cl}(t))(\delta x)^2\right] , \tag{3.52}$$

so the fluctuations are harmonic and the integrand on the right side of (3.52) has the form of an harmonic oscillator with the time dependent frequency $\Omega^2(t) = V''(x_{\rm cl}(t))/M$. The corresponding path integration can be carried out, yielding

$$\begin{aligned} F(x_b, t_b; x_a, t_a) &= \int_{x(t_a)=x_a}^{x(t_b)=x_b} \mathcal{D}\delta x(t)\, \exp\left\{\frac{i}{\hbar}\int_{t_a}^{t_b} dt\, \frac{M}{2}\left[\delta\dot{x}^2 - \Omega^2(t)\delta x^2\right]\right\} \\ &= \sqrt{\frac{M}{2\pi\, i\hbar(t_b - t_a)}}\sqrt{\frac{\det\left(-\partial_t\right)}{\det\left(-\partial_t - \Omega^2(t)\right)}} \end{aligned} \tag{3.53}$$

for the fluctuation factor. The functional determinants in (3.53) can be calculated with the Gelfand-Yaglom method [22, Chapter 2.4]. The determinants are discretized and then Laplace expanded; this yields a difference equation which can then be solved.

In fact, as all information on the fluctuation determinant in (3.53) is contained in the classical orbit $x_{\rm cl}(t)$, and thus in the classical action, it can be shown that (3.53) reduces to

$$F(x_b, t_b; x_a, t_a) = \sqrt{\frac{1}{2\pi\, i\hbar}\frac{-\partial^2\mathcal{A}(x_b, t_b; x_a, t_a)}{\partial x_a \partial x_b}} . \tag{3.54}$$

From this we obtain the Van-Vleck-Pauli-Morette formula for the semiclassical expansion up to quadratic order of the time evolution amplitude. In D dimensions it is given by

$$(\mathbf{x}_b, t_b | \mathbf{x}_a, t_a) \approx \sqrt{\frac{1}{(2\pi\, i\hbar)^D}\det\left[-\frac{\partial^2\mathcal{A}(\mathbf{x}_b, t_b; \mathbf{x}_a, t_a)}{\partial \mathbf{x}_a \partial \mathbf{x}_b}\right]} \exp\left\{\frac{i}{\hbar}\mathcal{A}(\mathbf{x}_b, t_b; \mathbf{x}_a, t_a)\right\} . \tag{3.55}$$

3.4.2 Time Evolution Amplitude for the Harmonic Oscillator

In this section we will calculate the one dimensional time evolution amplitude (3.15) for the important case of an harmonic oscillator, following the derivation presented in [26, Chapter 2.7]. We note, that the Van-Vleck-Pauli-Morette formula (3.55) is exact in this case, as the Hamiltonian is quadratic in $\mathbf{p}$ and $\mathbf{x}$ and thus the arising integrations in (3.45) can be carried out without the need for a saddle point approximation.

For the sake of generality, we will couple the harmonic oscillator to a current $j(t)$ which acts as a source. The path integral in configuration space for this system is

$$(x_b, t_b|x_a, t_a)[j] = \int_{x(t_a)=x_a}^{x(t_b)=x_b} \mathcal{D}x \, \mathrm{e}^{i\mathcal{A}[x,j]/\hbar} \,, \tag{3.56}$$

with the classical action

$$\mathcal{A}[x, j] = \int_{t_a}^{t_b} dt \left\{ \frac{M}{2} \dot{x}^2(t) - \frac{M}{2} \omega^2 x^2(t) + j(t)\, x(t) \right\} . \tag{3.57}$$

According to the Van-Vleck-Pauli-Morette formula (3.55), we must evaluate the action (3.57) along the classical path $x_{\text{cl}}(t)$ of the particle, which in turn is the set of all points where the classical action is stationary, i.e. (3.48), satisfying the boundary conditions $x_{\text{cl}}(t_a) = x_a$ and $x_{\text{cl}}(t_b) = x_b$. Carrying out the functional derivative in (3.48) yields the linear inhomogeneous second order differential equation of the harmonic oscillator:

$$\ddot{x}_{\text{cl}}(t) + \omega^2 x_{\text{cl}}(t) = \frac{j(t)}{M} \,. \tag{3.58}$$

Its general solution is a superposition of the solution $x_{\text{hom}}(t)$ of the homogeneous equation and of a particular solution $x_{\text{part}}(t)$ of the inhomogeneous equation (3.58).

Since the homogeneous equation is just that of the harmonic oscillator, it has the well known solution

$$x_{\text{hom}}(t) = c_1 \cos(\omega t) + c_2 \sin(\omega t) \,. \tag{3.59}$$

The boundary conditions $x_{\text{hom}}(t_a) = x_a$ and $x_{\text{hom}}(t_b) = x_b$ for the homogeneous equation lead to $x_{\text{part}}(t_a) = x_{\text{part}}(t_b) = 0$ for the inhomogeneous equation. Including these yields the coefficients in (3.59). They read

$$c_1 = \frac{x_a \sin(\omega t_b) - x_b \sin(\omega t_a)}{\sin[\omega(t_b - t_a)]} \,, \qquad c_2 = \frac{x_b \cos(\omega t_a) - x_a \cos(\omega t_b)}{\sin[\omega(t_b - t_a)]} \,, \tag{3.60}$$

so the solution of the homogeneous equation is

$$x_{\text{hom}}(t) = \frac{x_b \sin[\omega(t - t_a)] + x_a \sin[\omega(t_b - t)]}{\sin[\omega(t_b - t_a)]} \,. \tag{3.61}$$

We obtain a particular solution of (3.58) in terms of its associated Green's function $G(t, t')$, reading

$$x_{\text{part}}(t) = \int_{t_a}^{t_b} dt' \, G(t, t') \, \frac{j(t')}{M} \,, \tag{3.62}$$

which solves the differential equation (3.58) with a delta function inhomogenity,

$$\left(\frac{\partial^2}{\partial t^2}+\omega^2\right)G(t,t')=\delta(t-t')\ , \tag{3.63}$$

with the boundary conditions $G(t_a,t')=G(t_b,t')=0$. For $t\neq t'$, equation (3.63) is solved by

$$G(t,t')=\begin{cases}A(t')\,\sin\left[\omega(t_b-t)\right] & \text{for } t>t'\\ B(t')\,\sin\left[\omega(t-t_a)\right] & \text{for } t<t'\end{cases}\ , \tag{3.64}$$

so, assuming that $G(t,t')$ is continuous at $t=t'$, this leads to the condition

$$A(t')\,\sin\left[\omega(t_b-t')\right]-B(t')\,\sin\left[\omega(t'-t_a)\right]=0\ . \tag{3.65}$$

Consequently, the first derivative $G'(t,t')$ is discontinuous at $t=t'$, and we may exploit this jump by integrating (3.63) over a small intervall around t', which yields the second equation

$$A(t')\,\cos\left[\omega(t_b-t')\right]+B(t')\,\cos\left[\omega(t'-t_a)\right]=-\frac{1}{\omega}\ . \tag{3.66}$$

The last two equations determine the unknown functions $A(t')$ and $B(t')$. They read

$$A(t')=-\frac{\sin\left[\omega(t'-t_a)\right]}{\omega\,\sin\left[\omega(t_b-t_a)\right]}\ ,\qquad B(t')=-\frac{\sin\left[\omega(t_b-t')\right]}{\omega\,\sin\left[\omega(t_b-t_a)\right]}\ . \tag{3.67}$$

Now we can finally write down the expression for the Green's function. It is

$$G(t,t')=-\frac{\Theta(t-t')\,\sin\left[\omega(t_b-t)\right]\,\sin\left[\omega(t'-t_a)\right]+\Theta(t'-t)\,\sin\left[\omega(t_b-t')\right]\,\sin\left[\omega(t-t_a)\right]}{\omega\,\sin\left[\omega(t_b-t_a)\right]}\ . \tag{3.68}$$

Collecting everything, the classical path $x_{\mathrm{cl}}(t)$ of the particle is given by

$$\begin{aligned}x_{\mathrm{cl}}(t)=&\frac{x_b\,\sin\left[\omega(t-t_a)\right]+x_a\,\sin\left[\omega(t_b-t)\right]}{\sin\left[\omega(t_b-t_a)\right]}-\frac{1}{M\omega\,\sin\left[\omega(t_b-t_a)\right]}\int_{t_a}^{t_b}dt'\,j(t')\\ &\times\Big\{\Theta(t-t')\,\sin\left[\omega(t_b-t)\right]\,\sin\left[\omega(t'-t_a)\right]+\Theta(t'-t)\,\sin\left[\omega(t_b-t')\right]\,\sin\left[\omega(t-t_a)\right]\Big\}\ .\end{aligned} \tag{3.69}$$

We now have to evaluate the action (3.57) along this trajectory. To this end we note, that the aforementioned action may be written as

$$\mathcal{A}(x_b,t_b;x_a,t_a)[j]=\frac{M}{2}\Big[\dot{x}_{\mathrm{cl}}(t_b)\,x_b-\dot{x}_{\mathrm{cl}}(t_a)\,x_a\Big]+\frac{1}{2}\int_{t_a}^{t_b}dt'\,j(t')\,x_{\mathrm{cl}}(t')\ , \tag{3.70}$$

where we have performed an integration by parts. To further resolve this expression, we still need the velocity $\dot{x}_{\mathrm{cl}}(t)$ at the endpoints t_a and t_b of the classical path. Differentiating (3.69) yields

$$\dot{x}_{\mathrm{cl}}(t_b)=\frac{\omega\,\left\{x_b\,\cos\left[\omega(t_b-t_a)\right]-x_a\right\}}{\sin\left[\omega(t_b-t_a)\right]}+\frac{1}{M\,\sin\left[\omega(t_b-t_a)\right]}\int_{t_a}^{t_b}dt'\,\sin\left[\omega(t'-t_a)\right]j(t') \tag{3.71}$$

and

$$\dot{x}_{\rm cl}(t_a) = \frac{\omega\,\left(x_b - x_a\,\cos\left[\omega(t_b-t_a)\right]\right)}{\sin\left[\omega(t_b-t_a)\right]} - \frac{1}{M\,\sin\left[\omega(t_b-t_a)\right]}\int_{t_a}^{t_b} dt'\,\sin\left[\omega(t_b-t')\right] j(t')\;, \tag{3.72}$$

and thus the classical action (3.57) along the classical trajectory reads

$$\begin{aligned}\mathcal{A}(x_b,t_b;x_a,t_a)[j] = {} & \frac{M\,\omega}{2\sin\left[\omega(t_b-t_a)\right]}\Big\{(x_b^2+x_a^2)\cos\left[\omega(t_b-t_a)\right] - 2x_b\,x_a\Big\} \\ & + \int_{t_a}^{t_b} dt\,x_{\rm hom}(t)\,j(t) + \frac{1}{2M}\int_{t_a}^{t_b} dt\int_{t_a}^{t_b} dt'\,G(t,t')\,j(t)\,j(t')\;. \end{aligned} \tag{3.73}$$

Finally, we may insert (3.73) into the Van-Vleck-Pauli-Morette formula to obtain the final expression for the time evolution amplitude

$$\begin{aligned}(x_b,t_b|x_a,t_a)[j] = {} & \sqrt{\frac{M\omega}{2\pi\,i\hbar\sin\left[\omega(t_b-t_a)\right]}}\exp\left\{\frac{iM\omega}{2\hbar}\left[\frac{(x_b^2+x_a^2)\cos\left[\omega(t_b-t_a)\right]-2x_b\,x_a}{\sin\left[\omega(t_b-t_a)\right]}\right]\right\} \\ & \times\exp\left\{\frac{i}{\hbar}\int_{t_a}^{t_b} dt\,x_{\rm hom}(t)\,j(t) + \frac{1}{2M}\int_{t_a}^{t_b} dt\int_{t_a}^{t_b} dt'\,G(t,t')\,j(t)\,j(t')\right\}\;. \end{aligned} \tag{3.74}$$

The Wick rotated analogue of (3.74) follows from the path integral expression for the imaginary-time evolution amplitude (3.46) of the harmonic oscillator

$$(x_b,\hbar\beta|x_a,)[j] = \int_{x(0)=x_a}^{x(\hbar\beta)=x_b} \mathcal{D}x\,{\rm e}^{-\mathcal{A}[x,j]/\hbar}\;, \tag{3.75}$$

where the action in (3.75) is the Euclidean action

$$\mathcal{A}[x,j] = \int_0^{\hbar\beta} d\tau\,\left\{\frac{M}{2}\dot{x}^2(\tau) + \frac{M}{2}\omega^2 x^2(\tau) - j(\tau)x(\tau)\right\}\;. \tag{3.76}$$

Otherwise, the derivation is along the same lines as above, yielding

$$\begin{aligned}(x_b,\hbar\beta|x_a,0)[j] = {} & \sqrt{\frac{M\omega}{2\pi\,\hbar\sinh\left(\hbar\beta\omega\right)}}\exp\left\{-\frac{M\omega}{2\hbar}\left[\frac{(x_b^2+x_a^2)\cosh\left(\hbar\beta\omega\right)-2x_b\,x_a}{\sinh\left(\hbar\beta\omega\right)}\right]\right\} \\ & \times\exp\left\{\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau\,x_{\rm hom}(\tau)\,j(\tau) + \frac{1}{2\hbar^2}\int_0^{\hbar\beta} d\tau\int_0^{\hbar\beta} d\tau'\,G_\omega^{(\rm D)}(\tau,\tau')\,j(\tau)\,j(\tau')\right\}\;. \end{aligned} \tag{3.77}$$

Here,

$$x_{\rm hom}(\tau) = \frac{x_b\sinh\left(\omega\tau\right) + x_a\sinh\left[\omega(\hbar\beta-\tau)\right]}{\sinh\left(\hbar\beta\omega\right)} \tag{3.78}$$

is the Wick rotated homogeneous solution of (3.58) and

$$\begin{aligned}G_\omega^{(\rm D)}(\tau,\tau') = {} & \frac{\hbar}{M\omega\,\sinh\left(\hbar\beta\omega\right)}\Big\{\Theta(\tau-\tau')\sinh\left[\omega(\hbar\beta-\tau)\right]\sinh\left(\omega\tau'\right) \\ & + \Theta(\tau'-\tau)\sinh\left[\omega(\hbar\beta-\tau')\right]\sinh\left(\omega\tau\right)\Big\} \end{aligned} \tag{3.79}$$

denotes the Wick rotated Green's function.

We note, that integrating out the remaining coordinate in (3.77) yields the partition function of the one-dimensional single-particle harmonic oscillator:

$$Z_1(\beta)[j] = \int_{-\infty}^{\infty} dx\,(x,\hbar\beta|x,0)[j]\,. \tag{3.80}$$

Thus, for vanishing currents $j(\tau) = 0$, we obtain for the density matrix of the harmonic oscillator

$$\varrho_1(x_b,x_a) = \frac{1}{Z_1(\beta)}\,(x_b,\hbar\beta|x_a,0) \tag{3.81}$$

the explicit expression

$$\varrho_1(x_b,x_a) = \sqrt{\frac{M\omega}{\pi\hbar}\tanh\left(\frac{\hbar\beta\omega}{2}\right)}\exp\left\{-\frac{M\omega}{2\hbar}\left[\frac{(x_b^2+x_a^2)\cosh(\hbar\beta\omega)-2x_b\,x_a}{\sinh(\hbar\beta\omega)}\right]\right\}, \tag{3.82}$$

which reduces to a Gaussian for equal initial and final coordinates $x = x_b = x_a$. Performing an integration over the remaining coordinate x then yields the explicit expression

$$Z_1(\beta) = \frac{1}{2\sinh(\hbar\beta\omega/2)}\,. \tag{3.83}$$

for the canonical partition function of the harmonic oscillator.

3.4.3 Canonical Partition Function for Harmonic Potentials

According to (3.19) the one-particle density matrix is given by a normalised imaginary time amplitude. This is also true for the N-particle density matrix. However, for many particle systems, we must now sandwich the imaginary time evolution operator between the (anti-) symmetrised many-particle states (2.42). For noninteracting particles, due to the additivity of the many particle Hamiltonian, the N-particle imaginary-time evolution amplitude (3.17) factorises into one-particle amplitudes:

$$(\mathbf{x}_{1b},\ldots,\mathbf{x}_{Nb},\tau_b|\mathbf{x}_{1a},\ldots,\mathbf{x}_{Na},\tau_a)^{(\epsilon)} = \frac{1}{N!}\sum_P \epsilon^{p(P)}(\mathbf{x}_{P(1)b},\ldots,\mathbf{x}_{P(N)b},\tau_b|\mathbf{x}_{1a},\ldots,\mathbf{x}_{Na},\tau_a) \tag{3.84}$$

$$= \frac{1}{N!}\sum_P \epsilon^{p(P)}(\mathbf{x}_{P(1)b},\tau_b|\mathbf{x}_{1a},\tau_a)\cdots(\mathbf{x}_{P(N)b},\tau_b|\mathbf{x}_{Na},\tau_a)\,, \tag{3.85}$$

where only the one-particle states of the many-particle bra are permuted, in accordance with (2.49). For the simplest many particle system with $N = 2$, i.e. for two particles, we have

$$\begin{aligned}(\mathbf{x}_{1b},\mathbf{x}_{2b},\tau_b|\mathbf{x}_{1a},\mathbf{x}_{2a},\tau_a)^{(\epsilon)} = \frac{1}{2}\Big[&(\mathbf{x}_{1b},\tau_b|\mathbf{x}_{1a},\tau_a)\,(\mathbf{x}_{2b},\tau_b|\mathbf{x}_{2a},\tau_a)\\ &+\epsilon\,(\mathbf{x}_{2b},\tau_b|\mathbf{x}_{1a},\tau_a)\,(\mathbf{x}_{1b},\tau_b|\mathbf{x}_{2a},\tau_a)\Big]\,.\end{aligned} \tag{3.86}$$

With this we obtain the corresponding two-particle partition function via the continuous trace of (3.86) for $\tau_a = 0$ and $\tau_b = \hbar\beta$, i.e. by the integration:

$$Z_2(\beta) = \int_{-\infty}^{\infty} d^D x_1 \int_{-\infty}^{\infty} d^D x_2 \, (\mathbf{x}_1, \mathbf{x}_2, \hbar\beta | \mathbf{x}_1, \mathbf{x}_2, 0)^{(\epsilon)} \, . \tag{3.87}$$

The integration of the first two one-particle amplitudes in (3.86) just yields a product of two partition functions (3.83), one for each amplitude. In the remaining two amplitudes, we may first use their invariance under imaginary-time translations (3.20) to shift the imaginary time argument of the left amplitude by $\hbar\beta$. Subsequently, we can make use of the group property (3.25), so that the second integral becomes

$$\int_{-\infty}^{\infty} d^D x_1 \int_{-\infty}^{\infty} d^D x_2 \, (\mathbf{x}_2, 2\hbar\beta | \mathbf{x}_1, \hbar\beta) \, (\mathbf{x}_1, \hbar\beta | \mathbf{x}_2, 0) = (\mathbf{x}_2, 2\hbar\beta | \mathbf{x}_2, 0) \, , \tag{3.88}$$

yielding a one-particle partition function (3.83) at double imaginary time. Thus, we obtain

$$Z_2(\beta) = \frac{1}{2} \Big[Z_1^2(\beta) + \epsilon \, Z_1(2\beta) \Big] \tag{3.89}$$

for the two-particle partition function.

The three-particle partition function then follows along the same lines, the main difference being that for three particles there are $3! = 6$ permutations instead of the two in (3.86), namely

$$\begin{aligned}
(\mathbf{x}_{1b}, \mathbf{x}_{2b}, \mathbf{x}_{3b}, \tau_b | \mathbf{x}_{1a}, \mathbf{x}_{2a}, \mathbf{x}_{3a}, \tau_a)^{(\epsilon)} = \frac{1}{3!} \Big[& (\mathbf{x}_{1b}, \tau_b | \mathbf{x}_{1a}, \tau_a) \, (\mathbf{x}_{2b}, \tau_b | \mathbf{x}_{2a}, \tau_a) \, (\mathbf{x}_{3b}, \tau_b | \mathbf{x}_{3a}, \tau_a) \\
+ \epsilon (\mathbf{x}_{1b}, \tau_b | \mathbf{x}_{1a}, \tau_a) \, (\mathbf{x}_{3b}, \tau_b | \mathbf{x}_{2a}, \tau_a) \, (\mathbf{x}_{2b}, \tau_b | \mathbf{x}_{3a}, \tau_a) & + \epsilon (\mathbf{x}_{2b}, \tau_b | \mathbf{x}_{1a}, \tau_a) \, (\mathbf{x}_{1b}, \tau_b | \mathbf{x}_{2a}, \tau_a) \, (\mathbf{x}_{3b}, \tau_b | \mathbf{x}_{3a}, \tau_a) \\
+ \epsilon (\mathbf{x}_{3b}, \tau_b | \mathbf{x}_{1a}, \tau_a) \, (\mathbf{x}_{2b}, \tau_b | \mathbf{x}_{2a}, \tau_a) \, (\mathbf{x}_{1b}, \tau_b | \mathbf{x}_{3a}, \tau_a) & + (\mathbf{x}_{3b}, \tau_b | \mathbf{x}_{1a}, \tau_a) \, (\mathbf{x}_{1b}, \tau_b | \mathbf{x}_{2a}, \tau_a) \, (\mathbf{x}_{2b}, \tau_b | \mathbf{x}_{3a}, \tau_a) \\
& + (\mathbf{x}_{2b}, \tau_b | \mathbf{x}_{1a}, \tau_a) \, (\mathbf{x}_{3b}, \tau_b | \mathbf{x}_{2a}, \tau_a) \, (\mathbf{x}_{1b}, \tau_b | \mathbf{x}_{3a}, \tau_a) \Big] \, .
\end{aligned} \tag{3.90}$$

The trace of (3.90), i.e.

$$Z_3(\beta) = \int_{-\infty}^{\infty} d^D x_1 \int_{-\infty}^{\infty} d^D x_2 \int_{-\infty}^{\infty} d^D x_3 \, (\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \hbar\beta | \mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, 0)^{(\epsilon)} \, , \tag{3.91}$$

then yields the three-particle partition function

$$Z_3(\beta) = \frac{1}{3!} \Big[Z_1^3(\beta) + 3 \, \epsilon \, Z_1(\beta) Z_1(2\beta) + 2 \, Z_1(3\beta) \Big] \, . \tag{3.92}$$

Here, in analogy to the two-particle case, the first term in the sum of (3.90) stems from the identity permutation $\left(\begin{smallmatrix}1&2&3\\1&2&3\end{smallmatrix}\right)$ and yields a product of three partition functions in (3.92). In the second, third and fourth term of (3.90), corresponding to the three permutations with one transposition, we have an integral of the type (3.88), in addition to a one-particle partition function. These yield the second term in the sum of (3.92). Finally, the last term in (3.92) comes from the two permutations $\left(\begin{smallmatrix}1&2&3\\2&3&1\end{smallmatrix}\right)$ and $\left(\begin{smallmatrix}1&2&3\\3&1&2\end{smallmatrix}\right)$, for which we have triple integrals of the type (3.88), respectively, yielding two one-particle partition functions at three fold imaginary time. When we examine the cycle structure of the permutations that yield the different contributions to the two- and three-particle partitions functions above, we make the

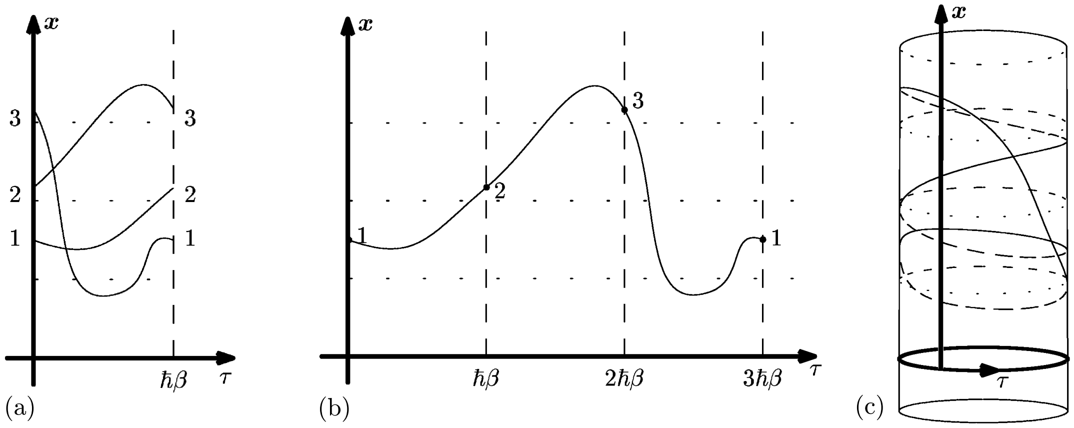

Figure 3.1: Example of the paths of three particles for a cycle of length $n = 3$ contributing to the partition function (3.93): (a) in the single-zone scheme, corresponding to the product of amplitudes $(\mathbf{x}_1, \hbar\beta|\mathbf{x}_2, 0)(\mathbf{x}_2, \hbar\beta|\mathbf{x}_3, 0)(\mathbf{x}_3, \hbar\beta|\mathbf{x}_1, 0)$, (b) the same situation in an extended zone scheme, corresponding to single amplitude $(\mathbf{x}_1, 3\hbar\beta|\mathbf{x}_2, 0)$ at a temperature that is scaled down by a factor of three, and (c) wrapped around an imaginary-time cylinder of circumference $\hbar\beta$.

following important observation: For the two-particle amplitude (3.86), the first product of two one-particle amplitudes on the right side corresponds to the identity permutation with the cycle structure (1)(2), i.e. it consists of two one-cycles, yielding a product of two one-particle partition functions in (3.89). In contrast, the second product of two one-particle amplitudes corresponds to a permutation which consists of the single *two-cycle* (12). This in turn yields a one-particle partition function at *double frequency* in the two-particle partition function (3.89), which we have printed in blue.

This pattern continues in the three-particle case: The identity permutation for three particles has the trivial cycle decomposition (1)(2)(3), and consequently this permutation yields a product of three one-particle partition functions in (3.92). In the three permutations (3)(12), (1)(23) and (2)(13), we have a *one-cycle* and a *two-cycle*, so these permutations each contribute a product of a single one-particle partition function with a one-particle partition function at double imaginary time. As in (3.89), we have printed the contribution of a two-cycle in blue. Finally, the two *three-cycle* permutations (231) and (312) each contribute a one-particle partition function, printed in green, at an imaginary time that is *three times* the original value.

Thus, the contributions to the many-particle partition functions come from the conjugation classes of the corresponding symmetric group. This does not come unexpectedly, as the original many particle states (2.42) are by construction invariant under the action of the symmetric group S_N.

Due to the indistinguishability of the particles, there are now one-particle amplitudes contributing to the partition function, whose final coordinates coincide with the initial coordinates of other particles, giving rise to many-particle formations, which are described by permutation cycles. Thus within these cycles, the particles change places with one another in a circular fashion. As an example, take the three amplitudes in (3.91) that correspond to a single three-cycle permutation, i.e. $(\mathbf{x}_1, \hbar\beta|\mathbf{x}_2, 0)(\mathbf{x}_2, \hbar\beta|\mathbf{x}_3, 0)(\mathbf{x}_3, \hbar\beta|\mathbf{x}_1, 0)$. Here, the particle at $\mathbf{x}_1$ goes to $\mathbf{x}_2$, the particle that was at $\mathbf{x}_2$ goes to $\mathbf{x}_3$, and the one at $\mathbf{x}_3$ goes to the original position of the first particle at $\mathbf{x}_1$. This situation is depicted in Fig. 3.1. In the first image (a), the three particle paths are displayed in a reduced zone scheme: Particle 1 does not arrive at its initial point after an imaginary time of $\tau = \hbar\beta$, but at the initial position of particle 2, which in turn arrives at the initial position of particle 3 at $\tau = \hbar\beta$. Furthermore, within the same imaginary time step, particle 3 goes to the starting point of particle 1, thus completing the cycle. Image (b) of Fig 3.1, depicts the same situation, but now in an extended zone scheme. The situation in (b) thus corresponds to the single imaginary time amplitude $(\mathbf{x}_1, 3\hbar\beta|\mathbf{x}_1, 0)$ at a temperature that is scaled down by a factor of three; in other words, it corresponds to a *single particle* going from $\mathbf{x}_1$ to $\mathbf{x}_1$ in an imaginary time $\tau = 3\hbar\beta$. Image (c) shows the "reduced" three-particle path wrapped around an imaginary-time cylinder of circumference $\hbar\beta$.

With the help of these insights, it is straightforward to generalise our derivation to the case of an N-particle ensemble. The trace of the (anti-) symmetrised N-particle amplitude (3.84) reads:

$$Z_N(\beta) = \frac{1}{N!}\sum_P \epsilon^{p(P)} \int_{-\infty}^{\infty} d^D x_1 \cdots \int_{-\infty}^{\infty} d^D x_N \, (\mathbf{x}_{P(1)}, \hbar\beta|\mathbf{x}_1, 0) \cdots (\mathbf{x}_{P(N)}, \hbar\beta|\mathbf{x}_N, 0) \; . \quad (3.93)$$

As we have seen above, the contribution of a single permutation cycle of length n to the N-particle partition function leads to an integral of the type

$$h_n(\beta) = \int_{-\infty}^{\infty} d^D x_1 \cdots \int_{-\infty}^{\infty} d^D x_n \, (\mathbf{x}_1, \hbar\beta|\mathbf{x}_n, 0)(\mathbf{x}_n, \hbar\beta|\mathbf{x}_{n-1}, 0) \cdots (\mathbf{x}_3, \hbar\beta|\mathbf{x}_2, 0)(\mathbf{x}_2, \hbar\beta|\mathbf{x}_1, 0) \; . \quad (3.94)$$

Using the imaginary time translation invariance (3.20), this can be brought into the form

$$h_n(\beta) = \int_{-\infty}^{\infty} d^D x_1 \cdots \int_{-\infty}^{\infty} d^D x_n \, (\mathbf{x}_1, n\hbar\beta|\mathbf{x}_n, (n-1)\hbar\beta)(\mathbf{x}_n, (n-1)\hbar\beta|\mathbf{x}_{n-1}, (n-2)\hbar\beta) \cdots (\mathbf{x}_3, 2\hbar\beta|\mathbf{x}_2, \hbar\beta)(\mathbf{x}_2, \hbar\beta|\mathbf{x}_1, 0) \; , \quad (3.95)$$

where we may now use the group property (3.25) of the one-particle amplitude to obtain

$$h_n(\beta) = \int_{-\infty}^{\infty} d^D x_1 \, (\mathbf{x}_1, n\hbar\beta|\mathbf{x}_1, 0) = Z_1(n\beta) \; . \quad (3.96)$$

With (3.94) and (3.96), we may rewrite the canonical N-particle partition function (3.93) as

$$Z_N(\beta) = \frac{1}{N!}\sum_P \epsilon^{p(P)} \prod_{n=1}^{\sum_n nC_n(P)=N} \Big[Z_1(n\beta)\Big]^{C_n(P)} \; . \quad (3.97)$$

Here, $C_n(P)$ is the number of n-cycles of the current permutation P. Instead of taking the number of n-cycles C_n to be a function of P, we may equally fix P by specifying the N-tuple of cycle numbers $(C_1, C_2, \ldots, C_N)$. In this cycle number notation, the sum over permutations in (3.97) can be rewritten in terms of a sum over all N-tuples that satisfy the condition $\sum_{n=1}^{N} nC_n = N$. In doing so, we must take into account that a certain N-tuple may occur multiple times in the permutation group, thus we must include a multiplicity factor $M(C_1, \ldots, C_N)$ in (3.97). With this, we obtain

$$Z_N(\beta) = \frac{1}{N!} \sum_{(C_1,\ldots,C_N)}^{\sum_n nC_n=N} \epsilon^{p(P)} M(C_1, \ldots, C_N) \prod_{n=1}^{\infty} \Big[Z_1(n\beta)\Big]^{C_n} \; , \quad (3.98)$$

where we have formally extended the product to all integers by setting $C_n = 0$ for all $n > N$, due to the condition $\sum_{n=1}^{N} nC_n = N$.

The derivation of the above multiplicity factor $M(C_1, \ldots, C_N)$ goes as follows: There are a total of $N!$ different N-tuples, corresponding to the order of the symmetric group S_N; however not all of these represent different permutations. According to Section 2.1.2, the following applies:

1. A cyclic permutation, i.e. a rotation of an n-cycle does not lead to a new permutation, so we have n irrelevant combinations for every n-cycle, or n^{C_n} irrelevant combinations for C_n n-cycles.
2. Reordering cycles of the same length does not lead to a new permutation, so for the number of C_n n-cycles we have $C_n!$ irrelevant combinations.

Thus, we obtain for the above multiplicity factor the Cauchy formula of the permutation group [18],

$$M(C_1, \ldots, C_N) = \frac{N!}{\prod_n C_n! n^{C_n}} \,. \tag{3.99}$$

Inserting (3.99) into (3.98) and observing that the parity $\epsilon^{p(P)}$ of a permutation P can be written as the product of the parities ϵ^{n+1} of individual n-cycles in (3.98), we finally arrive at the expression for the N-particle partition function in cycle reduced form:

$$Z_N(\beta) = \sum_{(C_1,\ldots,C_N)}^{\sum_n nC_n = N} \prod_{n=1}^{\infty} \frac{1}{C_n!} \left[\epsilon^{n+1} \frac{Z_1(n\beta)}{n} \right]^{C_n} \,. \tag{3.100}$$

The cycle representation (3.100) allows us to calculate the canonical partition function for any number of particles. In practice, however, this approach is not feasible for large particle numbers N as the computational effort grows with $N!$. Additionally, it is not straightforward to figure out all cycle numbers C_n which satisfy the condition $\sum_n nC_n = N$, so a more efficient algorithm for determining canonical partition functions is needed [28]. As a starting point in this direction, we note that the grand canonical partition function is the generating function of all canonical partition functions.

If we define the *fugacity* by $z = \mathrm{e}^{\beta\mu}$, with the chemical potential μ, the grand canonical partition function reads

$$\mathcal{Z}(\beta, z) = \sum_{N=0}^{\infty} Z_N(\beta)\, z^N \,. \tag{3.101}$$

This serves as the generating function of canonical partition functions which we obtain by Taylor-expanding (3.101), yielding the $Z_N(\beta)$ as expansion coefficients:

$$Z_N(\beta) = \frac{1}{N!} \frac{\partial^N}{\partial z^N} \mathcal{Z}(\beta, z) \bigg|_{z=0} \,. \tag{3.102}$$

In order to evaluate (3.101), we insert the cycle representation (3.100) and rewrite the exponent of the fugacity z using $N = \sum_n nC_n$. Thus, we have

$$\mathcal{Z}(\beta, z) = \sum_{N=0}^{\infty} \sum_{(C_1,\ldots,C_N)}^{\sum_n nC_n = N} \prod_{n=1}^{\infty} \frac{1}{C_n!} \left[\epsilon^{n+1} \frac{Z_1(n\beta)\, z^n}{n} \right]^{C_n} \tag{3.103}$$

in a first step. As in the above expression we are summing over all particle numbers from zero to infinity, we may drop the condition $\sum_n nC_n = N$ and instead sum over all cycle numbers from 0 to ∞, yielding

$$\mathcal{Z}(\beta, z) = \sum_{C_1=0}^{\infty} \sum_{C_2=0}^{\infty} \cdots \prod_{n=1}^{\infty} \frac{1}{C_n!} \left[\epsilon^{n+1} \frac{Z_1(n\beta)\, z^n}{n} \right]^{C_n} . \tag{3.104}$$

We may write this more compactly by rewriting the multiple sum over cycle numbers as a product over the individual sums, i.e.

$$\mathcal{Z}(\beta, z) = \prod_{n=1}^{\infty} \sum_{C_n=0}^{\infty} \frac{1}{C_n!} \left[\epsilon^{n+1} \frac{Z_1(n\beta)\, z^n}{n} \right]^{C_n} . \tag{3.105}$$

The C_n sum is an exponential, so we have

$$\mathcal{Z}(\beta, z) = \exp \left\{ \sum_{n=1}^{\infty} \epsilon^{n+1} \frac{Z_1(n\beta)\, z^n}{n} \right\} . \tag{3.106}$$

From (3.102) and (3.106) we find that the partition function of the vacuum, where no particles are present, i.e. $N = 0$, is given simply by

$$Z_0(\beta) = 1 . \tag{3.107}$$

Going on with our task of finding an alternative expression for the canonical partition function, we observe, that for $N \geq 1$ the grand canonical partition function (3.106) obeys the differential equation

$$\frac{\partial}{\partial z} \mathcal{Z}(\beta, z) = \mathcal{Z}(\beta, z) \sum_{k=1}^{\infty} Z_1(k\beta)\, z^{k-1} , \tag{3.108}$$

which we may solve recursively. To that end, we first form the Nth derivative of (3.101) via the Leibnitz rule of differentiation,

$$\left. \frac{\partial^N}{\partial z^N} \mathcal{Z}(\beta, z) \right|_{z=0} = \sum_{n=0}^{N} \frac{(N-1)!}{(n-1)!(N-n)!} \left. \frac{\partial^{N-n}}{\partial z^{N-n}} \mathcal{Z}(\beta, z) \right|_{z=0} \times \sum_{k=1}^{\infty} Z_1(k\beta) \left. \frac{\partial^{n-1} z^{k-1}}{\partial z^{n-1}} \right|_{z=0} , \tag{3.109}$$

and take into account that for the $(n-1)$st derivative of z^{k-1} in the rightmost sum of equation (3.109) we have the identity

$$\frac{\partial^{n-1} z^{k-1}}{\partial z^{n-1}} = (k-1)(k-2) \cdots (k-n+1) z^{k-n} = \begin{cases} \frac{(k-1)!}{(k-n)!} z^{k-n} & \text{for } k \geq n \\ 0 & \text{for } 1 \leq k < n \end{cases} . \tag{3.110}$$

With this, (3.109) reduces to

$$\frac{\partial^N}{\partial z^N} \mathcal{Z}(\beta, z) = (N-1)! \sum_{n=1}^{N} \frac{1}{(N-n)!} \frac{\partial^{N-n}}{\partial z^{N-n}} \mathcal{Z}(\beta, z) \frac{1}{(n-1)!} \sum_{k=1}^{\infty} Z_1(k\beta) \frac{(k-1)!}{(k-n)!} z^{k-n} . \tag{3.111}$$

Finally, taking (3.111) at $z = 0$ yields

$$\left.\frac{\partial^N}{\partial z^N}\mathcal{Z}(\beta,z)\right|_{z=0} = (N-1)!\sum_{n=1}^{N}\frac{\epsilon^{n+1}}{(N-n)!}\left.\frac{\partial^{N-n}}{\partial z^{N-n}}\mathcal{Z}(\beta,z)\right|_{z=0} Z_1(n\beta)\ , \tag{3.112}$$

and using (3.102) leaves us with the following recursion relation for the canonical partition functions $Z_N(\beta)$:

$$Z_N(\beta) = \frac{1}{N}\sum_{n=1}^{N}\epsilon^{n+1}Z_1(n\beta)Z_{N-n}(\beta)\ . \tag{3.113}$$

We note, that even though (3.113) is better suited for calculating the canonical partition function, its numerical evaluation possesses some additional difficulties: In (3.113) products of partition functions of different particle numbers N appear. For low enough temperatures we would thus be multiplying very small numbers with larger ones, which is not feasible due to the issues with numerical precision when computing with floating point numbers. However, this problem can be circumvented by rewriting and rescaling (3.113) in a suitable way [28].

3.5 Ideal Quantum Gases in Grand-Canonical Ensemble

We now turn to the description of ideal quantum gases in the grand canonical ensemble. The grand canonical formalism is considerably more popular with the BEC community, as it allows one to obtain analytical results for the different thermodynamic quantities, which do not involve the (anti) symmetrised many particle states (2.42). Thus, by working in the grand canonical ensemble, the considerable complications due to the permutation group can be avoided. In the thermodynamic limit of an infinitely large system, both the canonical and the grand canonical description coincide, whereas for finite, and particularly for small particle numbers, there can be significant deviations between both.

The starting point for the calculation of the grand canonical partition function $\mathcal{Z}(\beta)$ is the trace (3.11) of the grand canonical density operator (3.10). Here, it turns out to be best when one works in the formalism of the so called "second quantisation", i.e. with a field-theoretic approach, where in Fourier space the Hamiltonian and the particle number operator read

$$\hat{H} = \sum_{\mathbf{k}} E_{\mathbf{k}}\hat{n}_{\mathbf{k}}\ , \qquad \hat{N} = \sum_{\mathbf{k}}\hat{n}_{\mathbf{k}}\ , \tag{3.114}$$

respectively, with the occupation number operator $\hat{n}_{\mathbf{k}} = \hat{b}^+_{\mathbf{k}}\hat{b}_{\mathbf{k}}$, which is given in terms of the bosonic creation and anihilation operators (2.94) and (2.97). As we are dealing with ideal particle, there is no interaction, and consequently the Hamiltonian in (3.114) is additive in the single particle Hamiltonians. Here, the index $\mathbf{k}$ is a shorthand for all quantum numbers that are associated with the specific single-particle state. The trace of the partition function is then most conveniently carried out in the eigenbasis of $\hat{n}_{\mathbf{k}}$, namely in the discrete or occupation number basis of Fock space (2.91), that was introduced in Section 2.3.2. With this we have

$$\mathcal{Z}(\beta) = \mathrm{Tr}\left\{\mathrm{e}^{-\beta\sum_{\mathbf{k}}(E_{\mathbf{k}}-\mu)\hat{n}_{\mathbf{k}}}\right\} = \sum_{N}\sum_{n_{\mathbf{k}}}\langle N; n_1, n_2, \ldots|\,\mathrm{e}^{-\beta\sum_{\mathbf{k}}(E_{\mathbf{k}}-\mu)\hat{n}_{\mathbf{k}}}\,|N; n_1, n_2, \ldots\rangle\ . \tag{3.115}$$

Thus, grand canonically, a certain microstate in the ensemble, i.e. the corresponding quantum state is characterised by specifying the occupation numbers $(n_{\mathbf{k}}) = (n_1, n_2, n_3, \dots)$ of the single-particle states that are specified by $\mathbf{k}$.

With (3.115) the grand-canonical partition function (3.12) then reads

$$\mathcal{Z}(\beta) = \sum_N \sum_{n_{\mathbf{k}}} \mathrm{e}^{-\beta \sum_{\mathbf{k}} (E_{\mathbf{k}} - \mu) n_{\mathbf{k}}} = \sum_N \sum_{n_{\mathbf{k}}} \prod_{\mathbf{k}} \mathrm{e}^{-\beta (E_{\mathbf{k}} - \mu) n_{\mathbf{k}}} \, . \tag{3.116}$$

We note, that the occupation numbers in the first equation of (3.116) still sum up to a fixed particle number, that is, they obey the condition

$$N = \sum_{\mathbf{k}} n_{\mathbf{k}} \, , \tag{3.117}$$

which is simply the eigenvalue of the particle number operator in (3.114) and this is the reason for the additional N sum in equations (3.115) and (3.116). We may now also get rid of this sum, by observing that we can "generate" the quantum states of the system with arbitrary total particle number N, by exchanging in (3.116) the $n_{\mathbf{k}}$ sum and the product. Thus, the grand canonical partition function factorises into a product of one-particle partition functions:

$$\mathcal{Z}(\beta) = \prod_{\mathbf{k}} \left[\sum_{n_{\mathbf{k}}} \mathrm{e}^{-\beta (E_{\mathbf{k}} - \mu) n_{\mathbf{k}}} \right] \, . \tag{3.118}$$

This result is valid both for bosons and fermions. The different statistic for these two particle species manifest themselves in the conditions imposed on the respective occupation numbers $n_{\mathbf{k}}$, as we found in Section 2.3.2.

In the case of an ensemble of ideal bosons, the sum in (3.118) is a geometric series, which yields

$$\mathcal{Z}(\beta) = \prod_{\mathbf{k}} \left[1 - \mathrm{e}^{-\beta (E_{\mathbf{k}} - \mu)} \right]^{-1} \, . \tag{3.119}$$

For fermions, inserting $n_{\mathbf{k}} = 0, 1$ into (3.118) then gives us

$$\mathcal{Z}(\beta) = \prod_{\mathbf{k}} \left[1 + \mathrm{e}^{-\beta (E_{\mathbf{k}} - \mu)} \right] \, , \tag{3.120}$$

and we may then combine both cases into a single formula by writing

$$\mathcal{Z}(\beta) = \prod_{\mathbf{k}} \left[1 - \epsilon \, \mathrm{e}^{-\beta (E_{\mathbf{k}} - \mu)} \right]^{\epsilon} \, . \tag{3.121}$$

As an example for a thermodynamic expectation value in the grand canonical ensemble, let us calculate the important case of the expectation of the occupation number $n_{\mathbf{k}}$: From (3.118) we first have

$$\langle n_{\mathbf{k}} \rangle = \frac{1}{\mathcal{Z}(\beta)} \prod_{\mathbf{k}'} \left[\sum_{n_{\mathbf{k}'}} \mathrm{e}^{-\beta (E_{\mathbf{k}'} - \mu) n_{\mathbf{k}'}} \right] n_{\mathbf{k}} \, , \tag{3.122}$$

where we may pull out the single factor with $\mathbf{k}' = \mathbf{k}$, thus factorising the product in (3.122):

$$\langle n_{\mathbf{k}} \rangle = \frac{1}{\mathcal{Z}(\beta)} \prod_{\mathbf{k}' \neq \mathbf{k}} \left[\sum_{n_{\mathbf{k}'}} \mathrm{e}^{-\beta (E_{\mathbf{k}'} - \mu) n_{\mathbf{k}'}} \right] \sum_{n_{\mathbf{k}}} n_{\mathbf{k}} \mathrm{e}^{-\beta (E_{\mathbf{k}} - \mu) n_{\mathbf{k}}} \, . \tag{3.123}$$

Now, the sum over $n_{\mathbf{k}}$ is easily evaluated via a partial derivative of the partition function,

$$\sum_{n_{\mathbf{k}}} n_{\mathbf{k}} \mathrm{e}^{-\beta(E_{\mathbf{k}}-\mu)n_{\mathbf{k}}} = -\frac{1}{\beta}\frac{\partial}{\partial E_{\mathbf{k}}} \sum_{n_{\mathbf{k}}} \mathrm{e}^{-\beta(E_{\mathbf{k}}-\mu)n_{\mathbf{k}}} \;, \tag{3.124}$$

so, by using (3.14), (3.123) reduces to

$$\langle n_{\mathbf{k}} \rangle = -\frac{1}{\beta \mathcal{Z}(\beta)} \frac{\partial}{\partial E_{\mathbf{k}}} \mathcal{Z}(\beta) \;. \tag{3.125}$$

With this, we finally obtain the mean particle number

$$\langle n_{\mathbf{k}} \rangle = \frac{1}{\mathrm{e}^{-\beta(E_{\mathbf{k}}-\mu)} - \epsilon} \;, \tag{3.126}$$

which for bosons represents the Bose-Einstein and for fermions the Fermi-Dirac distribution function.

Chapter 4

Quench Dynamics of Harmonically Trapped Ideal Quantum Gases

In this Chapter we consider the problem of an ideal quantum gas of N particles, confined within a harmonic trap, with time-dependent trap frequency $\omega(t)$. The trapping potential is then that of the harmonic oscillator

$$V(x,t) = \frac{M}{2}\omega^2(t)\,x^2 \quad . \tag{4.1}$$

In the following, we restrict ourselves to the case of a quench, that is, a sudden change of trap frequency, at time t_a (see Fig. 4.2):

$$\omega(t) = \begin{cases} \omega & \text{for } t < t_a \\ \Omega & \text{for } t \geq t_a \,. \end{cases} \tag{4.2}$$

This is one of the simplest possible non-equilibrium problems and we expect the quantum gas to respond to the quench with some kind of oscillatory behaviour. To this end, we work out expressions for the time-dependent density matrix and for the reduced one-particle density matrix, since the latter is related to the condensate's density function and is thus a quantity that can be experimentally observed.

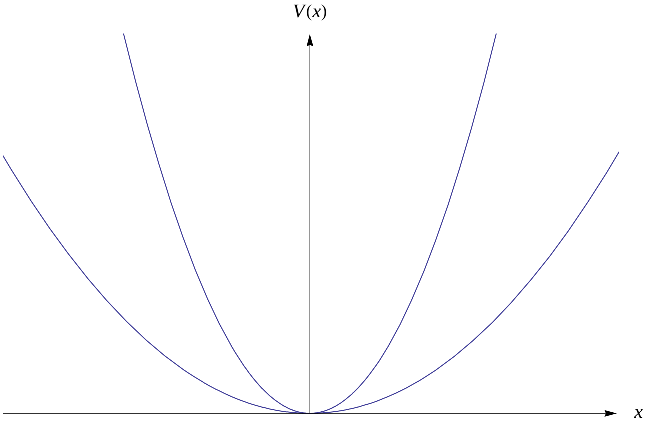

Figure 4.1: Harmonic potential $V(x)$ for trap frequencies ω and Ω.

4.1 One-Particle Time Dependent Density Matrix

In standard quantum mechanics and for a general time-dependent Hamiltonian $\hat{H}(t)$, a density operator $\hat{\varrho}$, which is taken to be in the Schrödinger picture, evolves in time according to the *von Neumann equation*

$$i\hbar \frac{\partial}{\partial t}\hat{\varrho} = \left[\hat{H}(t), \hat{\varrho}\right] , \tag{4.3}$$

which is analoguous to the *Liouville equation* in classical physics. Equation (4.3) is solved by

$$\hat{\varrho}(t_b) = \hat{U}(t_b, t_a)\ \hat{\varrho}(t_a)\ \hat{U}^{-1}(t_b, t_a) , \tag{4.4}$$

where the unitary time evolution operator $\hat{U}(t_b, t_a)$ is formally given by the Dyson series

$$\hat{U}(t_b, t_a) = \hat{T}\ \exp\left\{-\frac{i}{\hbar}\int_{t_a}^{t_b} dt'\ \hat{H}(t')\right\} , \tag{4.5}$$

and where $\hat{T}$ denotes the time-ordering operator. For the simpler case of a time-independent Hamiltonian, e.g. for the time-dependence (4.2), the time-evolution operator reduces to $\hat{U}(t_b, t_a) = \exp\{-i\hat{H}_\Omega(t_b - t_a)/\hbar\}$, and the time-evolution of the density operator reads

$$\hat{\varrho}(t_b) = \mathrm{e}^{-\frac{i}{\hbar}\hat{H}_\Omega(t_b - t_a)}\ \hat{\varrho}(t_a)\ \mathrm{e}^{+\frac{i}{\hbar}\hat{H}_\Omega(t_b - t_a)} . \tag{4.6}$$

We obtain the corresponding density matrix by going to the standard coordinate basis, i.e. by sandwiching $\hat{\varrho}(t_b)$ between position eigenstates $\langle x_b|$ and $|x_{b'}\rangle$:

$$\varrho_1(x_b, x_{b'}; t_b) = \langle x_b| e^{-\frac{i}{\hbar}\hat{H}_\Omega(t_b - t_a)}\ \hat{\varrho}(t_a)\ e^{+\frac{i}{\hbar}\hat{H}_\Omega(t_b - t_a)}|x_{b'}\rangle. \tag{4.7}$$

We have given the density matrix an index 1 to clarify that it represents a one-particle quantity, and note, that the underlying Hamiltonian in coordinate representation reads

$$\hat{H}_\Omega = -\frac{\hbar^2}{2M}\frac{d^2}{dx^2} + \frac{M}{2}\Omega^2 x^2 . \tag{4.8}$$

For fixed x_b, $x_{b'}$ the expression above is an amplitude and we may insert the identity operator $\hat{\mathbb{1}}$ twice in form of the completeness relation

$$\hat{\mathbb{1}} = \int dx_a |x_a\rangle\langle x_a| \tag{4.9}$$

for x_a and $x_{a'}$, respectively, obtaining

$$\varrho_1(x_b, x_{b'}; t_b) = \int dx_a \int dx_{a'} (x_b, t_b|x_a, t_a)\, \varrho_1(x_a, x_{a'}; t_a)\, (x_{a'}, t_a|x_{b'}, t_b) . \tag{4.10}$$

Here the time evolution is described by the real-time evolution amplitude

$$(x_b, t_b|x_a, t_a) = \langle x_b|\, e^{-\frac{i}{\hbar}\hat{H}_\Omega(t_b - t_a)}\, |x_a\rangle . \tag{4.11}$$

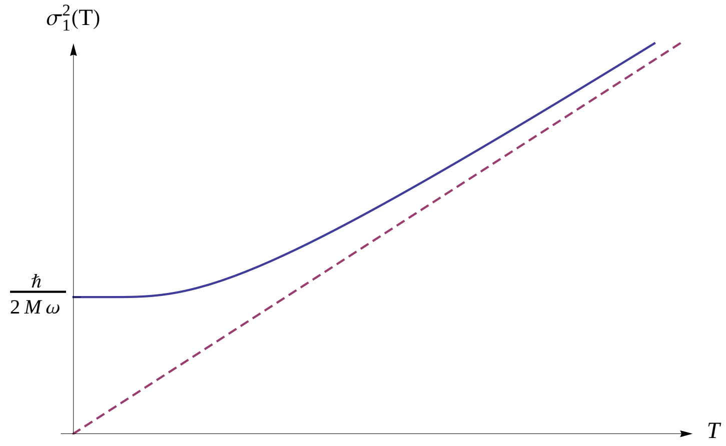

Figure 4.2: Harmonic oscillator equilibrium width $\sigma^2(T)$ together with its asymptote (dashed) which correspond to the law of Dulong Petit.

Our initial condition is the density matrix of the one-particle harmonic oscillator, $\varrho_1(x_a, x_{a'}; t_a)$, at initial time t_a, that was calculated from the semi-classical expansion of the path-integral in Section 3.4 and which is given in Wick-rotated imaginary time as

$$\varrho_1(x_a, x_{a'}; t_a) = \sqrt{\frac{M\omega}{\pi\hbar}\tanh\left(\frac{\hbar\beta\omega}{2}\right)}\exp\left\{-\frac{M\omega}{2\hbar}\left[\frac{\left(x_a^2+x_{a'}^2\right)\cosh\left(\hbar\beta\omega\right)-2x_a x_{a'}}{\sinh\left(\hbar\beta\omega\right)}\right]\right\}. \tag{4.12}$$

Thus, by using the above ansatz, we completely separate the (imaginary time) equilibrium dynamics from the non-equilibrium dynamics (real time) in parameter space. The full time-dependent non-equilibrium density matrix for the one-particle harmonic oscillator is then given by equation (4.10), where

$$(x_b, t_b|x_a, t_a) = \sqrt{\frac{M\Omega}{2\pi\, i\hbar\sin\left[\Omega\left(t_b-t_a\right)\right]}}\exp\left\{\frac{iM\Omega}{2\,\hbar}\left[\frac{\left(x_b^2+x_a^2\right)\cos\left[\Omega\left(t_b-t_a\right)\right]-2\,x_b x_a}{\sin\left[\Omega\left(t_b-t_a\right)\right]}\right]\right\} \tag{4.13}$$

and

$$(x_{a'}, t_a|x_{b'}, t_b) = \sqrt{\frac{M\Omega}{2\pi\, i\hbar\sin\left[\Omega\left(t_a-t_b\right)\right]}}\exp\left\{\frac{iM\Omega}{2\,\hbar}\left[\frac{\left(x_{a'}^2+x_{b'}^2\right)\cos\left[\Omega\left(t_a-t_b\right)\right]-2\,x_{a'} x_{b'}}{\sin\left[\Omega\left(t_a-t_b\right)\right]}\right]\right\} \tag{4.14}$$

are the corresponding real-time forward- and backward-evolution amplitudes, respectively. After inserting (4.12)–(4.14), we may rewrite (4.10) as the two-dimensional Gaussian integral

$$\varrho_1(x_b, x_{b'}; t_b) = \sqrt{\frac{M^3\Omega^2\omega\tanh\left(\hbar\beta\omega/2\right)}{4\pi^3\hbar^3\sin^2\left[\Omega(t_b-t_a)\right]}}\exp\left\{\frac{iM\Omega(x_b^2-x_{b'}^2)\cot\left[\Omega(t_b-t_a)\right]}{2\hbar}\right\}$$
$$\times\int_{-\infty}^{\infty} d^2x_a\exp\left\{-\mathbf{x}^\dagger A\mathbf{x}-\mathbf{b}^\dagger\mathbf{x}\right\}, \tag{4.15}$$

with the abbreviation $d^2x_a = dx_a dx_{a'}$, and with the matrix A and constant vector $\mathbf{b}^\dagger$ given by

$$\mathbf{b}^\dagger = -i\frac{M\Omega}{\hbar\sin\left[\Omega\left(t_b-t_a\right)\right]}\begin{pmatrix}-x_b\\ +x_{b'}\end{pmatrix} ,$$
$$A = \begin{pmatrix}\dfrac{M\omega}{2\hbar}\coth\left(\hbar\beta\omega\right) - \dfrac{iM\Omega}{2\hbar}\cot\left[\Omega(t_b-t_a)\right] & -\dfrac{M\omega}{2\hbar\sinh\left(\hbar\beta\omega\right)}\\ -\dfrac{M\omega}{2\hbar\sinh\left(\hbar\beta\omega\right)} & \dfrac{M\omega}{2\hbar}\coth\left(\hbar\beta\omega\right) + \dfrac{iM\Omega}{2\hbar}\cot\left[\Omega(t_b-t_a)\right]\end{pmatrix} . \tag{4.16}$$

Using the formula for multi-dimensional Gaussian integrals

$$\int_{-\infty}^{\infty} d^N x \, \exp\left\{-\mathbf{x}^\dagger A\mathbf{x} + \mathbf{b}^\dagger\mathbf{x}\right\} = \sqrt{\frac{\pi^N}{\det\left(A\right)}}\exp\left\{\frac{1}{4}\mathbf{b}^\dagger A^{-1}\mathbf{b}\right\} , \tag{4.17}$$

we obtain the following expression for the time-dependent one-particle harmonic density matrix:

$$\varrho_1(x_b, x_{b'}; t_b) = \sqrt{\frac{M\omega\tanh\left(\hbar\beta\omega/2\right)}{\pi\hbar f(t_b-t_a)}}\exp\left\{\frac{-M\omega}{2\hbar f(t_b-t_a)}\left[\frac{(x_b^2+x_{b'}^2)\cosh\left(\hbar\beta\omega\right) - 2x_b x_{b'}}{\sinh\left(\hbar\beta\omega\right)}\right]\right\} . \tag{4.18}$$

Comparing (4.18) above with the initial thermodynamic time-independent density matrix (4.12), we note that the former differs from the latter only by the factor

$$f(t_b-t_a) = \frac{\omega^2\sin^2\left[\Omega\left(t_b-t_a\right)\right] + \Omega^2\cos^2\left[\Omega\left(t_b-t_a\right)\right]}{\Omega^2} , \tag{4.19}$$

which is present both in the prefactor and in the exponential. Note that if we set $\Omega = \omega$ in (4.18), it reduces to the time-independent expression (4.12). Equally, when setting $t_b - t_a = 0$, it reduces to (4.12), as expected.

The diagonal elements of (4.18) are Gaussian distributed and, as expected, setting $x_{b'} = x_b$ yields

$$\varrho_1(x_b, x_b; t_b) = \sqrt{\frac{2M\omega\tanh\left(\hbar\beta\omega/2\right)}{2\pi\,\hbar\,f(t_b-t_a)}}\exp\left\{-\frac{2M\omega}{2\pi\,\hbar\,f(t_b-t_a)}\tanh\left(\hbar\beta\omega/2\right)x_b^2\right\} , \tag{4.20}$$

which has the form of a Gaussian,

$$\frac{1}{\sqrt{2\pi\sigma^2}}\exp\left\{-\frac{x^2}{2\sigma^2}\right\} , \tag{4.21}$$

with width

$$\sigma_1^2(t_b, t_a; T) = \frac{\hbar}{2M\omega}\coth\left(\hbar\beta\omega/2\right)\left(\frac{\omega^2\sin^2\left[\Omega\left(t_b-t_a\right)\right] + \Omega^2\cos^2\left[\Omega\left(t_b-t_a\right)\right]}{\Omega^2}\right) . \tag{4.22}$$

The factor in front is $\hbar/(2M\omega) = x_0^2/2$ where x_0 is the well-known oscillator width, which is a measure for the typical length scale of the system. We note that when setting $\Omega = \omega$, (4.22) becomes time-independent and we obtain the equilibrium width $\sigma_1^2(T) = (\hbar/2M\omega)\coth\left(\hbar\beta\omega/2\right)$ as expected.

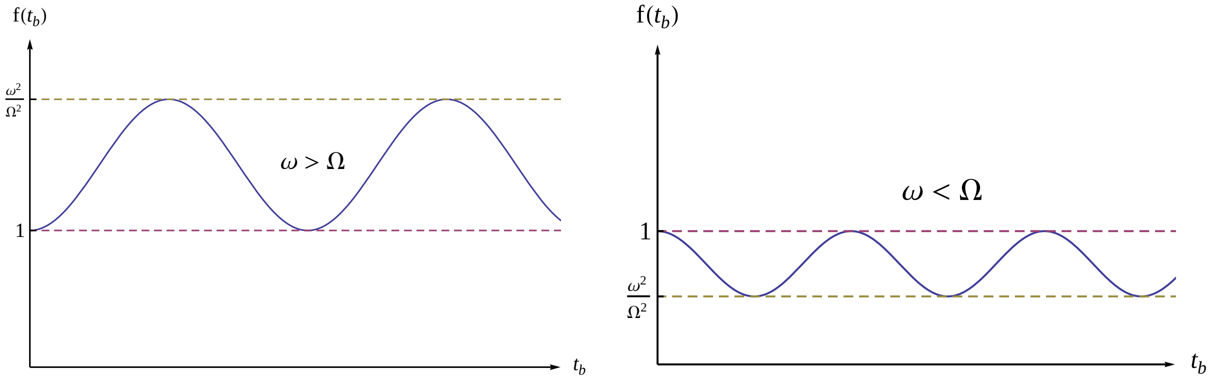

Figure 4.3: Oscillatory behaviour of the time-dependence function $f(t_b - t_a)$ for $\omega > \Omega$ (left) and $\omega < \Omega$ (right).

As is depicted in Fig. 4.2, $\sigma^2(T)$ grows linearly with T sufficiently large, corresponding to the law of Dulong Petit, and departs from this asymptote for $T \approx 0$, approaching $\hbar/(2M\omega)$, as dictated by the uncertainty relation. We also note that (4.22) may be written as a product

$$\sigma_1^2(t;T) = \sigma_1^2(0;T) f(t_b - t_a) \;, \tag{4.23}$$

where $\sigma_1^2(0;T) \equiv \sigma_1^2(T)$, and for $t_a = 0$, we may rewrite $f(t_b)$ as

$$f(t_b) = \frac{1}{2}\left(1 + \frac{\omega^2}{\Omega^2}\right) + \frac{1}{2}\left(1 - \frac{\omega^2}{\Omega^2}\right)\cos\left(2\Omega t_b\right) \;, \tag{4.24}$$

which oscillates between 1 and ω^2/Ω^2 as is illustrated in Fig. 4.3.

4.2 Two-Particle Time Dependent Density Matrix

In this section we extend our ansatz from the previous section to the case of two particles, taking into account that we now have a true many-particle system. Consequently, as we are dealing with identical particles, we must sandwich our two-particle density operator between (anti-) symmetrized two-particle position eigenstates. The many-particle position eigenstates (2.79) were introduced in Section 2.3.1

Following the procedure for the one-particle case, we insert two two-particle completeness relations of the form (2.80) and, pulling out the normalisation factor $1/Z_2(\beta)$ from the two-particle density matrix, rewrite our expression for the two-particle time-dependent non-equilibrium density matrix as

$$\begin{aligned}\varrho_2(x_{1b}, x_{2b}; x_{1b'}, x_{2b'}; t_b) = \frac{1}{Z_2(\beta)} \int dx_{1a} \int dx_{2a} \int dx_{1a'} \int dx_{2a'}\, (x_{1b}, x_{2b}; t_b | x_{1a}, x_{2a}; t_a)^{(\epsilon)} \\ \times (x_{1a}, x_{2a}; \tau_a | x_{1a'}, x_{2a'}; \tau_{a'})^{(\epsilon)}\, (x_{1a'}, x_{2a'}; t_a | x_{1b'}, x_{2b'}; t_b)^{(\epsilon)} \;. \end{aligned} \tag{4.25}$$

The three properly (anti-)symmetrized two-particle amplitudes amplitudes read as follows:

$$\begin{aligned}(x_{1b}, x_{2b}; t_b | x_{1a}, x_{2a}; t_a)^{\epsilon} = \frac{1}{2!}\Big[(x_{1b}, t_b | x_{1a}, t_a)\, (x_{2b}, t_b | x_{2a}, t_a) \\ + \epsilon\, (x_{1b}, t_b | x_{2a}, t_a)\, (x_{2b}, t_b | x_{1a}, t_a) \Big] \;, \end{aligned} \tag{4.26}$$

$$
\begin{aligned}
(x_{1a}, x_{2a}; \tau_a | x_{1a'}, x_{2a'}; \tau_{a'})^{\epsilon} = \frac{1}{2!} \Big[& (x_{1a}, \tau_a | x_{1a'}, \tau_{a'})\, (x_{2a}, \tau_a | x_{2a'}, \tau_{a'}) \\
& + \epsilon\, (x_{1a}, \tau_a | x_{2a'}, \tau_{a'})\, (x_{2a}, \tau_a | x_{1a'}, \tau_{a'}) \Big] \,,
\end{aligned} \tag{4.27}
$$

$$
\begin{aligned}
(x_{1a'}, x_{2a'}; t_a | x_{1b'}, x_{2b'}; t_b)^{\epsilon} = \frac{1}{2!} \Big[& (x_{1a'}, t_a | x_{1b'}, t_b)\, (x_{2a'}, t_a | x_{2b'}, t_b) \\
& + \epsilon\, (x_{1a'}, t_a | x_{2b'}, t_b)\, (x_{2a'}, t_a | x_{1b'}, t_b) \Big] \,,
\end{aligned} \tag{4.28}
$$

They factorise into products of one-particle amplitudes (4.13) and (4.14), as we are dealing with ideal, i.e. non-interacting particles.

We see that the situation is already more complicated for the two-particle case, as we must now take into account that the particles are quantum objects which are naturally indistinguishable. As it was said in Section 2.3, the amplitudes are subject to (anti-) symmetrisation, and for two particles there are the two possible permutations of coordinates displayed in (4.26)–(4.28), resulting in a sum of two terms in every two-particle amplitude. Putting these into (4.25), we get

$$
\begin{aligned}
\varrho_2(x_{1b}, x_{2b}; x_{1b'}, x_{2b'}; t_b) = {} & \frac{1}{Z_2(\beta)} \frac{1}{8} \int dx_{1a} \int dx_{2a} \int dx_{1a'} \int dx_{2a'} \\
& \times \Big[(x_{1b}, t_b | x_{1a}, t_a)\, (x_{2b}, t_b | x_{2a}, t_a) + \epsilon\, (x_{1b}, t_b | x_{2a}, t_a)\, (x_{2b}, t_b | x_{1a}, t_a) \Big] \\
& \times \Big[(x_{1a}, \tau_a | x_{1a'}, \tau_{a'})\, (x_{2a}, \tau_a | x_{2a'}, \tau_{a'}) + \epsilon\, (x_{1a}, \tau_a | x_{2a'}, \tau_{a'})\, (x_{2a}, \tau_a | x_{1a'}, \tau_{a'}) \Big] \\
& \times \Big[(x_{1a'}, t_a | x_{1b'}, t_b)\, (x_{2a'}, t_a | x_{2b'}, t_b) + \epsilon\, (x_{1a'}, t_a | x_{2b'}, t_b)\, (x_{2a'}, t_a | x_{1b'}, t_b) \Big] \,,
\end{aligned} \tag{4.29}
$$

and multiplying out gives the following eight terms

$$
\begin{aligned}
= {} & \frac{1}{Z_2(\beta)} \frac{1}{8} \int dx_{1a} \int dx_{2a} \int dx_{1a'} \int dx_{2a'} \\
& \Big[(x_{1b}, t_b | x_{1a}, t_a)\, (x_{2b}, t_b | x_{2a}, t_a)\, (x_{1a}, \tau_a | x_{1a'}, \tau_{a'})\, (x_{2a}, \tau_a | x_{2a'}, \tau_{a'})\, (x_{1a'}, t_a | x_{1b'}, t_b)\, (x_{2a'}, t_a | x_{2b'}, t_b) \\
& + \epsilon\ \, (x_{1b}, t_b | x_{1a}, t_a)\, (x_{2b}, t_b | x_{2a}, t_a)\, (x_{1a}, \tau_a | x_{1a'}, \tau_{a'})\, (x_{2a}, \tau_a | x_{2a'}, \tau_{a'})\, (x_{1a'}, t_a | x_{2b'}, t_b)\, (x_{2a'}, t_a | x_{1b'}, t_b) \\
& + \epsilon\ \, (x_{1b}, t_b | x_{1a}, t_a)\, (x_{2b}, t_b | x_{2a}, t_a)\, (x_{1a}, \tau_a | x_{2a'}, \tau_{a'})\, (x_{2a}, \tau_a | x_{1a'}, \tau_{a'})\, (x_{1a'}, t_a | x_{1b'}, t_b)\, (x_{2a'}, t_a | x_{2b'}, t_b) \\
& + \epsilon^2 (x_{1b}, t_b | x_{1a}, t_a)\, (x_{2b}, t_b | x_{2a}, t_a)\, (x_{1a}, \tau_a | x_{2a'}, \tau_{a'})\, (x_{2a}, \tau_a | x_{1a'}, \tau_{a'})\, (x_{1a'}, t_a | x_{2b'}, t_b)\, (x_{2a'}, t_a | x_{1b'}, t_b) \\
& + \epsilon\ \, (x_{1b}, t_b | x_{2a}, t_a)\, (x_{2b}, t_b | x_{1a}, t_a)\, (x_{1a}, \tau_a | x_{1a'}, \tau_{a'})\, (x_{2a}, \tau_a | x_{2a'}, \tau_{a'})\, (x_{1a'}, t_a | x_{1b'}, t_b)\, (x_{2a'}, t_a | x_{2b'}, t_b) \\
& + \epsilon^2 (x_{1b}, t_b | x_{2a}, t_a)\, (x_{2b}, t_b | x_{1a}, t_a)\, (x_{1a}, \tau_a | x_{1a'}, \tau_{a'})\, (x_{2a}, \tau_a | x_{2a'}, \tau_{a'})\, (x_{1a'}, t_a | x_{2b'}, t_b)\, (x_{2a'}, t_a | x_{1b'}, t_b) \\
& + \epsilon^2 (x_{1b}, t_b | x_{2a}, t_a)\, (x_{2b}, t_b | x_{1a}, t_a)\, (x_{1a}, \tau_a | x_{2a'}, \tau_{a'})\, (x_{2a}, \tau_a | x_{1a'}, \tau_{a'})\, (x_{1a}, t_a | x_{1b'}, t_b)\, (x_{2a'}, t_a | x_{2b'}, t_b) \\
& + \epsilon^3 (x_{1b}, t_b | x_{2a}, t_a)\, (x_{2b}, t_b | x_{1a}, t_a)\, (x_{1a}, \tau_a | x_{2a'}, \tau_{a'})\, (x_{2a}, \tau_a | x_{1a'}, \tau_{a'})\, (x_{1a'}, t_a | x_{2b'}, t_b)\, (x_{2a'}, t_a | x_{1b'}, t_b) \Big] \,.
\end{aligned} \tag{4.30}
$$

Using the relation

$$
Z_1(\beta)\, \varrho_1(x_{1b}, x_{1b'}; t_b) = \int dx_{1a} \int dx_{1a'}\, (x_{1b}, t_b | x_{1a}, t_a)\, (x_{1a}, \tau_a | x_{1a'}, \tau_{a'})\, (x_{1a'}, t_a | x_{1b'}, t_b) \ , \tag{4.31}
$$

which follows from the definition of the one-particle density matrix (4.18), we can now rearrange and combine terms and obtain the following expression for the non-equilibrium, two-particle density matrix:

$$\varrho_2(x_{1b}, x_{2b}; x_{1b'}, x_{2b'}; t_b) = \frac{Z_1^2(\beta)}{Z_2(\beta)} \frac{1}{2} \Big[\varrho_1(x_{1b}, x_{1b'}; t_b)\, \varrho_1(x_{2b}, x_{2b'}; t_b) + \epsilon\, \varrho_1(x_{1b}, x_{2b'}; t_b)\, \varrho_1(x_{2b}, x_{1b'}; t_b) \Big] . \tag{4.32}$$

4.3 Two-Particle Partition Function

Our next task is to check that $\varrho_2(x_{1b}, x_{2b}; x_{1b'}, x_{2b'}; t_b)$ is normalised, i.e. that integrating out all coordinates of (4.32) yields the two-particle partition function $Z_2(\beta)$. We set $x_{1b} = x_{1b'}$ and $x_{2b} = x_{2b'}$, use (4.12), and integrate over both coordinates:

$$Z_2(\beta) = \frac{Z_1^2(\beta)}{2} \frac{M\omega \tanh(\hbar\beta\omega/2)}{\pi\hbar f(t_b - t_a)} \Bigg[\int dx_{1b} \int dx_{2b} \exp\left\{ -\frac{M\omega \tanh(\hbar\beta\omega/2)}{\hbar f(t_b - t_a)} \left(x_{1b}^2 + x_{2b}^2\right) \right\} + \epsilon \int dx_{1b} \int dx_{2b} \exp\left\{ -\frac{M\omega}{\hbar f(t)} \left[\frac{(x_{1b}^2 + x_{2b}^2)\cosh(\hbar\beta\omega) - x_{1b}x_{2b}}{\sinh(\hbar\beta\omega)} \right] \right\} \Bigg] . \tag{4.33}$$

The first integral in (4.33) is straightforward to calculate, since it is a simple Gaussian. The second integral can be written as a two-dimensional Gaussian integral (4.17) without the linear term. The off-diagonal terms in the corresponding matrix must be distributed symmetrically, since multidimensional Gaussian integrals are defined only for symmetric matrix exponentials. The symmetrised matrix A reads

$$A = \begin{pmatrix} a & -b \\ -b & a \end{pmatrix} , \tag{4.34}$$

with the abbreviations

$$a = \left[\frac{M\omega}{\hbar f(t_b - t_a)} \right] \coth(\hbar\beta\omega) \qquad b = \left[\frac{M\omega}{\hbar f(t_b - t_a)} \right] \frac{1}{\sinh(\hbar\beta\omega)} . \tag{4.35}$$

Its determinant is given by

$$\det(A) = a^2 - b^2 = \left[\frac{M\omega}{\hbar f(t_b - t_a)} \right]^2 \frac{\cosh^2(\hbar\beta\omega) - 1}{\sinh^2(\hbar\beta\omega)} = \left[\frac{M\omega}{\hbar f(t_b - t_a)} \right]^2 . \tag{4.36}$$

When we insert the solution, according to (4.17), of the second integral into (4.33), we may pull out the time-dependent factor from the square brackets, cancelling the same factor in front. We get

$$Z_2(\beta) = \frac{1}{2} \Big[Z_1^2(\beta) + \epsilon\, Z_1^2(\beta)\, \tanh(\hbar\beta\omega/2) \Big] . \tag{4.37}$$

Here we may now use $\sinh(x) = 2\sinh(x/2)\cosh(x/2)$ and the expression for the canonical one-particle partition function (3.83), to obtain

$$Z_2(\beta) = \frac{1}{2} \Big[Z_1^2(\beta) + \epsilon\, Z_1(2\beta) \Big] , \tag{4.38}$$

which is the correct expression for the two-particle harmonic oscillator partition function from (3.89).

4.4 One-Particle Time Dependent Reduced Density Matrix in Two-Particle Ensemble

We now turn to the computation of the reduced one-particle density matrix in a two-particle ensemble, $\varrho_2^{(\mathrm{r})}(x_{1b}, x_{1b'}; t_b)$, which is a one-particle quantity, i.e. a function of the first particle's coordinates. We obtain it by tracing out the degrees of freedom of the second particle, thus including the effects of the second particle on particle number one. Here we have chosen the coordinates of particle number one to be left out from integration, but this choice is without loss of generality, as we are always free to change the overall numbering of particle coordinates when we are dealing with indistinguishable particles. In order to simplify a later generalisation to N particles, it is useful to observe that the two permutations of coordinates in (4.32), i.e. $P_1 = \left(\begin{smallmatrix}1 & 2\\ 1 & 2\end{smallmatrix}\right)$ and $P_2 = \left(\begin{smallmatrix}1 & 2\\ 2 & 1\end{smallmatrix}\right)$, have the cycle-decomposition (1)(2) and (12), i.e. the first consists of two one-cycles and the latter of one two-cycle, and that we are effectively *breaking* the two-cycle in (4.32), by setting the second particle's coordinates equal, $x_{2b} = x_{2b'}$, and leaving $x_{1b} \neq x_{1b'}$.

$$\varrho_1^{(\mathrm{r})}(x_{1b}, x_{1b'}; t) = \frac{Z_1^2(\beta)}{Z_2(\beta)} \frac{1}{2} \Big[\varrho_1(x_{1b}, x_{1b'}; t_b) \underbrace{\int dx_{2b}\, \varrho_1(x_{2b}, x_{2b'}; t_b)}_{=1} + \epsilon \int dx_{2b}\, \underbrace{\varrho_1(x_{1b}, x_{2b}; t_b)\, \varrho_1(x_{2b}, x_{1b'}; t_b)}_{\text{broken two-cycle}} \Big] \tag{4.39}$$

In order to evaluate (4.39) further, we must find a way to integrate products of one-particle density matrices that correspond to broken cycles. To this end we will integrate the simplest non-trivial broken n-cycle, namely the broken two-cycle in (4.39), i.e. $\varrho_1(x_{1b}, x_{2b}; t_b)\varrho_1(x_{2b}, x_{1b'}; t_b)$, and derive a master integral that may be later on applied to the integration of a general broken n-cycle. In order to apply this master integral to a general n-cycle later, we will be more general with the two-cycle, and take the two one-particle density matrices at different imaginary time, β and β':

$$\begin{aligned} &Z_1(\beta)Z_1(\beta') \int_{-\infty}^{\infty} dx_{2b}\; \varrho_1(x_{1b}, x_{2b}; t_b, \beta)\varrho_1(x_{2b}, x_{1b'}; t_b, \beta') \\ &= \frac{\sqrt{\tanh(\hbar\beta\omega/2)\tanh(\hbar\beta'\omega/2)}}{4\sinh(\hbar\beta\omega/2)\sinh(\hbar\beta'\omega/2)} \frac{M\omega}{\pi\hbar f(t_b - t_a)} \int_{-\infty}^{\infty} dx_{2b} \\ &\quad \times \exp\left\{ -\frac{M\omega}{2\hbar f(t_b - t_a)} \left[x_{1b}^2 \coth(\hbar\beta\omega) + x_{2b}^2 \coth(\hbar\beta\omega) - 2\frac{x_{1b}x_{2b}}{\sinh(\hbar\beta\omega)} \right] \right\} \\ &\quad \times \exp\left\{ -\frac{M\omega}{2\hbar f(t_b - t_a)} \left[x_{1b}^2 \coth(\hbar\beta'\omega) + x_{2b}^2 \coth(\hbar\beta'\omega) - 2\frac{x_{1b}x_{2b}}{\sinh(\hbar\beta'\omega)} \right] \right\} . \end{aligned} \tag{4.40}$$

Performing the Gaussian integral yields

$$
\begin{aligned}
=&\frac{\sqrt{\tanh(\hbar\beta\omega/2)\tanh(\hbar\beta'\omega/2)}}{4\sinh(\hbar\beta\omega/2)\sinh(\hbar\beta'\omega/2)}\sqrt{\frac{1}{\coth(\hbar\beta\omega)+\coth(\hbar\beta'\omega)}}\sqrt{\frac{2M\omega}{\pi\hbar f(t_b-t_a)}}\\
&\times\exp\left\{-\frac{M\omega}{2\hbar f(t_b-t_a)}\left[x_{1b}^2\coth(\hbar\beta\omega)+x_{1b'}^2\coth(\hbar\beta'\omega)\right]\right\}\\
&\times\exp\left\{-\frac{M\omega}{2\hbar f(t_b-t_a)}\left[\frac{x_{1b}}{\sinh(\hbar\beta\omega)}+\frac{x_{1b'}}{\sinh(\hbar\beta'\omega)}\right]^2\left[\frac{1}{\coth(\hbar\beta\omega)+\coth(\hbar\beta'\omega)}\right]\right\}.
\end{aligned}
\tag{4.41}
$$

Before going on, let us simplify the prefactor of the exponentials in the first line of (4.41). Step by step we get

$$
\frac{\sqrt{\tanh(\hbar\beta\omega/2)\tanh(\hbar\beta'\omega/2)}}{4\sinh(\hbar\beta\omega/2)\sinh(\hbar\beta'\omega/2)}\sqrt{\frac{1}{\coth(\hbar\beta\omega)+\coth(\hbar\beta'\omega)}}\sqrt{\frac{2M\omega}{\pi\hbar f(t_b-t_a)}}
\tag{4.42}
$$

$$
\begin{aligned}
=&\sqrt{\frac{2M\omega}{\pi\hbar f(t_b-t_a)}}\sqrt{\frac{\sinh(\hbar\beta\omega/2)\sinh(\hbar\beta'\omega/2)}{\cosh(\hbar\beta\omega/2)\cosh(\hbar\beta'\omega/2)}}\frac{1}{4\sinh(\hbar\beta\omega/2)\sinh(\hbar\beta'\omega/2)}\\
&\times\sqrt{\frac{4\sinh(\hbar\beta\omega/2)\sinh(\hbar\beta'\omega/2)\cosh(\hbar\beta\omega/2)\cosh(\hbar\beta'\omega/2)}{\cosh(\hbar\beta\omega)\sinh(\hbar\beta'\omega)+\cosh(\hbar\beta'\omega)\sinh(\hbar\beta\omega)}}
\end{aligned}
\tag{4.43}
$$

$$
=\sqrt{\frac{M\omega}{2\pi\hbar f(t_b-t_a)}}\sqrt{\frac{1}{\sinh[\hbar\omega(\beta+\beta')]}}\,.
\tag{4.44}
$$

Now we can continue with the exponentials. After expanding the fractions in the argument of the first and second exponential of (4.41), we have

$$
\begin{aligned}
&Z_1(\beta)Z_1(\beta')\int_{-\infty}^{\infty}dx_{2b}\;\varrho_1(x_{1b},x_{2b};t_b,\beta)\varrho_1(x_{2b},x_{1b'};t_b,\beta')=\\
&=\sqrt{\frac{M\omega}{2\pi\hbar f(t_b-t_a)}}\sqrt{\frac{1}{\sinh[\hbar\omega(\beta+\beta')]}}\\
&\times\exp\left\{-\frac{M\omega}{2\hbar f(t_b-t_a)}\left[\frac{x_{1b}^2\cosh(\hbar\beta\omega)\sinh(\hbar\beta'\omega)+x_{1b'}^2\cosh(\hbar\beta'\omega)\sinh(\hbar\beta\omega)}{\sinh(\hbar\beta\omega)\sinh(\hbar\beta'\omega)}\right]\right\}\\
&\times\exp\left\{\frac{M\omega}{2\hbar f(t_b-t_a)}\left[\frac{x_{1b}^2\sinh^2(\hbar\beta'\omega)+x_{1b'}^2\sinh^2(\hbar\beta\omega)+2x_{1b}x_{1b'}\sinh(\hbar\beta\omega)\sinh(\hbar\beta'\omega)}{\sinh(\hbar\beta\omega)\sinh(\hbar\beta'\omega)\sinh[\hbar\omega(\beta+\beta')]}\right]\right\}.
\end{aligned}
\tag{4.45}
$$

Taking the common denominator in both exponentials of (4.41), and collecting separately the prefactors of x_{1b}^2 and $x_{1b'}^2$, yields

$$\begin{aligned}
&= \sqrt{\frac{M\omega}{2\pi\hbar f(t_b-t_a)}}\sqrt{\frac{1}{\sinh\left[\hbar\omega(\beta+\beta')\right]}} \\
&\times \exp\left\{\frac{M\omega}{2\hbar f(t_b-t_a)}\left[x_{1b}^2\left(\frac{\sinh^2(\hbar\beta'\omega)-\cosh^2(\hbar\beta\omega)\sinh^2(\hbar\beta'\omega)-(1/4)\sinh(2\hbar\beta\omega)\sinh(2\hbar\beta'\omega)}{\sinh(\hbar\beta\omega)\sinh(\hbar\beta'\omega)\sinh\hbar\omega(\beta+\beta')}\right)\right.\right. \\
&\left.\left. + x_{1b'}^2\left(\frac{\sinh^2(\hbar\beta\omega)-\cosh^2(\hbar\beta'\omega)\sinh^2(\hbar\beta\omega)-(1/4)\sinh(2\hbar\beta\omega)\sinh(2\hbar\beta'\omega)}{\sinh(\hbar\beta\omega)\sinh(\hbar\beta'\omega)\sinh\left[\hbar\omega(\beta+\beta')\right]}\right) + \frac{2\,x_{1b}\,x_{1b'}}{\sinh\left[\hbar\omega(\beta+\beta')\right]}\right]\right. .
\end{aligned} \tag{4.46}$$

We may now use the hyperbolic Pythagoras' theorem $\cosh^2(\hbar\beta\omega)-\sinh^2(\hbar\beta\omega)=1$ for β and β' in the prefactor of x_{1b}^2 and $x_{1b'}^2$. Now two pairs of hyperbolic sines cancel in every prefactor, one with primed and one with unprimed beta, and we are left with

$$\begin{aligned}
&= \sqrt{\frac{M\omega}{\pi\hbar f(t_b-t_a)}\frac{1}{4\tanh\left[\hbar\omega\left(\beta+\beta'\right)/2\right]}} \\
&\qquad\qquad \times \exp\left\{-\frac{M\omega}{2\hbar f(t_b-t_a)}\left[\frac{(x_{1b}^2+x_{1b'}^2)\cosh\left[\hbar\omega(\beta+\beta')\right]-2\,x_{1b}\,x_{1b'}}{\sinh\left[\hbar\omega(\beta+\beta')\right]}\right]\right\}
\end{aligned} \tag{4.47}$$

$$= Z_1(\beta+\beta')\,\varrho_1\left(x_{1b},x_{1b'};t_b,(\beta+\beta')\right) \ , \tag{4.48}$$

where we have used the double angle formula $\sinh(2x)=2\sinh(x)\cosh(x)$ and have expanded the fraction in the square root of the overall prefactor. In the next step, we may now use our master equation

$$Z_1(\beta)Z_1(\beta')\int_{-\infty}^{\infty}dx_{2b}\;\varrho_1(x_{1b},x_{2b};t_b,\beta)\varrho_1(x_{2b},x_{1b'};t_b,\beta') = Z_1(\beta+\beta')\varrho_1\left(x_{1b},x_{1b'};t_b,(\beta+\beta')\right) \ , \tag{4.49}$$

to evaluate the above expression for the one-particle reduced density matrix (4.39). We obtain

$$\varrho_1^{(\mathrm{r})}(x_{1b},x_{1b'};t) = \frac{1}{Z_2(\beta)}\frac{1}{2}\Big[Z_1^2(\beta)\;\varrho_1(x_{1b},x_{1b'};t_b) + \epsilon\,Z_1(2\beta)\;\varrho_1(x_{1b},x_{1b'};t_b,2\beta)\Big] \ . \tag{4.50}$$

We are also interested in the expression for the one-particle width in a two-particle ensemble, since we would like to compare it to the corresponding one-particle width (4.22). Just as with the reduced one-particle density matrix above, in a two-particle ensemble we must include the effect of the environment on the particle of interest. Thus, we must take the thermodynamic expectation value of x_{1b}^2, but with the *reduced* one-particle density matrix (4.50) instead of (4.18). Consequently, the reduced one-particle width in a two-particle ensemble follows from its trace:

$$\sigma_1^{(\mathrm{r})2}(\beta) = \mathrm{Tr}\left\{\varrho_1^{(\mathrm{r})}(x_{1b},x_{1b'};t_b=0)\,x_{1b}^2\right\} = \frac{1}{Z_2(\beta)}\frac{1}{2}\left[\sigma_1^2(0,\beta)\;Z_1^2(\beta) + \epsilon\,\sigma_1^2(0,2\beta)\;Z_1(2\beta)\right] \ . \tag{4.51}$$

4.5 *N*-Particle Time Dependent Density Matrix

We will now generalise our calculation to the case of N ideal particles, following closely the path of the previous sections. In complete analogy to the one- and two-particle cases, we begin by multiplying the N-particle harmonic oscillator density operator with the N-particle time-evolution operator $\exp\{-\frac{i}{\hbar}(\hat{H}_\Omega^{(1)}+\hat{H}_\Omega^{(2)}+\cdots+\hat{H}_\Omega^{(N)})(t_b-t_a)\}$ from the left, and with its Hermitian conjugate from the right, and thereafter sandwiching the resulting time-dependent density operator between N-particle position eigenstates. When we insert two N-particle completeness relations (2.80), we know that we will end up with a product of three N-particle time-evolution amplitudes, as in (4.25) for the two-particle case, and with the inverse N-particle partition function $Z_N^{-1}(\beta)$ as the corresponding normalisation factor. Thus, our ansatz for the N-particle time dependent density matrix is

$$\varrho_N(x_{1b},\ldots,x_{Nb};x_{1b'},\ldots,x_{Nb'};t_b)=\frac{1}{Z_N(\beta)}\int d^Nx_a\int d^Nx_{a'}\,(x_{1b},\ldots,x_{Nb};t_b|x_{1a},\ldots,x_{Na};t_a)^{(\epsilon)}$$
$$\times\,(x_{1a},\ldots,x_{Na};\tau_a|x_{1a'},\ldots,x_{Na'};\tau_{a'})^{(\epsilon)}\,(x_{1a'},\ldots,x_{Na'};t_a|x_{1b'},\ldots,x_{Nb'};t_b)^{(\epsilon)}\ , \quad (4.52)$$

where we insert an (anti-)symmetrised imaginary-time evolution amplitude of the form (2.49), respective (2.48), i.e.

$$(x_{1b},\ldots,x_{Nb};t_b|x_{1a},\ldots,x_{Na};t_a)^{(\epsilon)}=\frac{1}{N!}\sum_P\epsilon^{p(P)}\Big[\big(x_{P(1)b},t_b|x_{1a},t_a\big)\cdots\big(x_{P(N)b},t_b|x_{Na},t_a\big)\Big] \quad (4.53a)$$

$$=\frac{1}{N!}\sum_P\epsilon^{p(P)}\Big[\big(x_{1b},t_b|x_{P(1)a},t_a\big)\cdots\big(x_{Nb},t_b|x_{P(N)a},t_a\big)\Big], \quad (4.53b)$$

expressed in terms of one-particle amplitudes, for each of the three N-particle amplitudes in equation (4.52). From (2.46)–(2.49) in Section 2.3.1 we know, that it makes no difference in (4.53), whether the permutation is in the left coordinate's index, as in (4.53a), or in the right coordinate's index as in (4.53b). We now substitute the above relation (4.53b) for the left real-time amplitude, and the other relation (4.53a) for the middle imaginary-time as well as the right-hand real-time amplitudes, respectively. With this we obtain

$$\varrho_N(x_{1b},\ldots,x_{Nb};x_{1b'},\ldots,x_{Nb'};t_b)=\frac{1}{Z_N(\beta)}\left(\frac{1}{N!}\right)^3\int d^Nx_a\int d^Nx_{a'}\sum_{P,P',P''}\epsilon^{p(P)+p(P')+p(P'')}$$
$$\times\Big[\big(x_{P(1)b};t_b|x_{1a};t_a\big)\,\big(x_{1a};\tau_a|x_{P'(1)a'};\tau_{a'}\big)\,\big(x_{1a'};t_a|x_{P''(1)b'};t_b\big)\cdots$$
$$\cdots\big(x_{P(N)b};t_b|x_{Na};t_a\big)\,\big(x_{Na};\tau_a|x_{P'(N)a'};\tau_{a'}\big)\,\big(x_{Na'};t_a|x_{P''(N)b'};t_b\big)\Big] \quad (4.54)$$

with the triple sum over the permutations P, P', P'', respectively. Note that we have rearranged the one-particle amplitudes in (4.54), so that we now have N groups of one-particle amplitudes, each one consisting of a real-time amplitude to the left, an imaginary-time amplitude in the centre, and another real-time amplitude to the right.

We will now fit the left coordinates of the respective right real-time amplitudes to the neighbouring P'-permuted coordinates of the imaginary-time amplitudes. In other words:

we permute the coordinates $x_{1a'}, \ldots, x_{Na'}$ according to P'. This has the effect of changing the right coordinates of the respective right real-time amplitude from $x_{P''(1)b'}, \ldots, x_{P''(N)b'}$ to $x_{P''(P'(1))b'}, \ldots, x_{P''(P'(N))b'}$. This change corresponds to a rearrangement of the right real-time amplitudes, so that their left coordinates correspond to the right coordinates of the unchanged imaginary-time amplitudes.

To clarify this procedure, consider the nth group of three one-particle amplitudes in (4.54):

$$\left(x_{P(n)b}; t \middle| \, x_{na}; 0\right) \left(x_{na}; \beta \middle| \, x_{P'(n)a'}; 0\right) \left(x_{na'}; 0 \middle| \, x_{P''(n)b'}; t\right) \tag{4.55}$$

We may use the relation (4.18), where the one-particle equilibrium density matrix is given as a normalised imaginary time amplitude

$$\varrho_1(x_b, x_{b'}; t_b) = \frac{1}{Z_1(\beta)} \left(x_b; \beta \middle| \, x_{b'}; 0\right) \ , \tag{4.56}$$

to write every group of amplitudes (4.55) as a time-dependent density matrix (4.18), if we can bring the above group into the required form. To this end, we make the opposing coordinates between two amplitudes equal. The opposing coordinates in the first two amplitudes from the left of (4.55) are already the same, so the second pair of coordinates remains. The suitable right amplitude for our three-group (4.55) certainly exists, since all permutations of coordinates appear in (4.54). It is the real-time amplitude where the left coordinate is permuted according to $P'(n)$, so its right coordinate must be permuted according to $P''(P'(n))$. Swapping the wrong right amplitude in (4.55) with the suitable one, we have

$$\left(x_{P(n)b}, t \middle| \, x_{na}, 0\right) \left(x_{na}, \beta \middle| \, x_{P'(n)a'}, 0\right) \left(x_{P'(n)a'}, 0 \middle| \, x_{P''(P'(n))b'}, t\right) \ , \tag{4.57}$$

which has the appropriate form. Carrying out this procedure for all N three-groups of amplitudes in (4.54), we arrive at

$$\begin{aligned} \varrho_N(x_{1b}, \ldots, x_{Nb}; x_{1b'}, \ldots, x_{Nb'}; t) = \frac{1}{Z_N(\beta)} \left(\frac{1}{N!}\right)^3 \int d^N x_a \int d^N x_{a'} \sum_{P,P',P''} \epsilon^{p(P)+p(P')+p(P'')} \\ \times \Big[\left(x_{P(1)b}; t_b | x_{1a}; t_a\right) \left(x_{1a}; \tau_a | x_{P'(1)a'}; \tau_{a'}\right) \left(x_{P'(1)a'}; t_a | x_{P''(P'(1))b'}; t_b\right) \cdots \\ \cdots \left(x_{P(N)b}; t_b | x_{Na}; t_a\right) \left(x_{Na}; \tau_a | x_{P'(N)a'}; \tau_{a'}\right) \left(x_{P'(N)a'}; t_a | x_{P''(P'(N))b'}; t_b\right) \Big] \ . \end{aligned} \tag{4.58}$$

Now, for $n = 1, \ldots, N$, we may write every group of three amplitudes as a one-particle density matrix (4.10) times a partition function:

$$\begin{aligned} Z_1(\beta)\, \varrho_1(x_{P(n)b}, x_{P''(P'(n))b'}; t_b) = \int dx_{na} \int dx_{P'(n)a'} \\ \times \left(x_{P(n)b}, t_b | x_{na}, t_a\right) \left(x_{na}, \tau_a | x_{P'(n)a'}, \tau_{a'}\right) \left(x_{P'(n)a'}, t_a | x_{P''(P'(n))b'}, t_b\right) \ . \end{aligned} \tag{4.59}$$

Defining $\tilde{P} = P''P'$ for the combination of permutations thus leads to

$$\begin{aligned} \varrho_N(x_{1b}, \ldots, x_{Nb}; x_{1b'}, \ldots, x_{Nb'}; t_b) = \frac{1}{Z_N(\beta)} \left(\frac{1}{N!}\right)^2 \sum_P \sum_{\tilde{P}} \epsilon^{p(P)+p(\tilde{P})} \\ \times \left[Z_1^N(\beta)\, \varrho_1\left(x_{P(1)b}, x_{\tilde{P}(1)b'}; t_b\right) \cdots \varrho_1\left(x_{P(N)b}, x_{\tilde{P}(N)b'}; t_b\right) \right] . \end{aligned} \tag{4.60}$$

We may now also get rid of another of the remaining two permutations, by permuting the N one-particle density matrices according to $\tilde{P}$, for example. This is possible, of course, as we may permute groups of one-particle amplitudes, as well as the amplitudes themselves:

$$\varrho_N(x_{1b},\ldots,x_{Nb};x_{1b'},\ldots,x_{Nb'};t_b) = \frac{Z_1^N(\beta)}{Z_N(\beta)}\left(\frac{1}{N!}\right)^2 \sum_P \sum_{\tilde{P}^{-1}} \epsilon^{p(P)+p(\tilde{P}^{-1})} \times \varrho_1(x_{P(\tilde{P}^{-1}(1))b},x_{1b'};t_b)\cdots\varrho_1(x_{P(\tilde{P}^{-1}(N))b},x_{Nb'};t_b). \quad (4.61)$$

We again define a composite permutation $\bar{P} = P\tilde{P}^{-1}$, and, dropping the superfluous sum over permutations $\tilde{P}$, as well as another factor of $1/N!$, arrive at the final expression for the N-particle density matrix

$$\varrho_N(x_{1b},\ldots,x_{Nb};x_{1b'},\ldots,x_{Nb'};t_b) = \frac{Z_1^N(\beta)}{Z_N(\beta)}\frac{1}{N!}\sum_{\bar{P}} \epsilon^{p(\bar{P})}\varrho_1(x_{\bar{P}(1)b},x_{1b'};t_b)\cdots\varrho_1(x_{\bar{P}(N)b},x_{Nb'};t_b) \quad (4.62)$$

in terms of one-particle density matrices and one-particle partition functions.

4.6 *N*-Particle Partition Function

We now turn to the partition function of our quenched ideal gas and note that – as the partition function is a time-independent quantity – we expect to recover the well-known expression for the partition function of the ideal gas, either in cycle reduced form (3.100), or as a recursion relation (3.113), thus taking the same road as for the one-particle and the two-particle cases in the previous Sections 4.1 and 4.3. We start with the normalisation condition for the N-particle density matrix (4.62),

$$1 = \int d^N x_b \; \varrho_N(x_{1b},\ldots,x_{Nb};x_{1b},\ldots,x_{Nb};t_b) \; . \quad (4.63)$$

We insert (4.62) and bring the normalisation factor to the left side. Then, performing the N-dimensional integration yields the following equation for the N-particle partition function in terms of an integral over a sum of permuted one-particle density matrices:

$$Z_N(\beta) = Z_1^N(\beta)\frac{1}{N!}\sum_P \epsilon^{p(P)}\int d^N x_b \; \varrho_1(x_{P(1)b},x_{1b};t_b)\cdots\varrho_1(x_{P(N)b},x_{Nb};t_b) \; . \quad (4.64)$$

Inserting (4.18), we obtain

$$Z_N(\beta) = Z_1^N(\beta)\frac{1}{N!}\sum_P \epsilon^{p(P)}\left[\frac{M\omega\,\tanh(\hbar\beta\omega/2)}{\pi\hbar f(t_b-t_a)}\right]^{N/2}\int d^N x_b \times \exp\left\{\frac{-M\omega}{\hbar f(t_b-t_a)}\left[\frac{\left(x_{1b}^2+\cdots+x_{Nb}^2\right)\cosh(\hbar\beta\omega)-\left(x_{1b}\,x_{P(1)b}+\cdots+x_{Nb}\,x_{P(N)b}\right)}{\sinh(\hbar\beta\omega)}\right]\right\}, \quad (4.65)$$

where we note that the expression $(x_{1b}^2+\cdots+x_{Nb}^2 \; + \; x_{P(1)b}^2+\cdots+x_{P(N)b}^2)$ in the exponent of (4.65) contains the sum of all squared coordinates twice, and we have pulled out a factor of

2 which cancels the factor 1/2 present in all one-particle density matrices (4.18). The integral in (4.65) can be written as an N-dimensional Gaussian

$$Z_N(\beta) = Z_1^N(\beta)\frac{1}{N!}\sum_P \epsilon^{p(P)}\left[\frac{M\omega\ \tanh(\hbar\beta\omega/2)}{\pi\hbar f(t_b-t_a)}\right]^{N/2}\int d^N x_b \exp\Big\{-\mathbf{x}^\dagger\mathbf{A}(P)\mathbf{x}\Big\}, \tag{4.66}$$

with the matrix $\mathbf{A}(P)$ depending on the permutation in the outer sum; i.e. we must sum over all possible permutations P, and – for every term in this sum – integrate a matrix exponential with a different matrix $\mathbf{A}$ corresponding to the respective permutation P. In the following, we will abbreviate the above expression by noting that the N-dimensional Gaussian above yields

$$\frac{\pi^{N/2}}{\sqrt{\det(\mathbf{A}(P))}}\,, \tag{4.67}$$

so our task is to construct the matrices $\mathbf{A}(P)$ and to find an expression for their determinants. To this end we write

$$\begin{aligned} Z_N(\beta) &= Z_1^N(\beta)\frac{1}{N!}\left[\frac{M\omega\ \tanh(\hbar\beta\omega/2)}{\hbar f(t_b-t_a)}\right]^{N/2} \\ &\times\sum_P \epsilon^{p(P)}\int d^N x_b\ \exp\left\{-a\left(x_{1b}^2+\cdots+x_{Nb}^2\right)+b\left(x_{1b}\,x_{P(1)b}+\cdots+x_{Nb}\,x_{P(N)b}\right)\right\} \end{aligned} \tag{4.68}$$

and obtain

$$Z_N(\beta) = Z_1^N(\beta)\frac{1}{N!}\left[\frac{M\omega\ \tanh(\hbar\beta\omega/2)}{\hbar f(t_b-t_a)}\right]^{\frac{N}{2}}\sum_P \epsilon^{p(P)}\left[\frac{\pi^N}{\det(\mathbf{A}(P))}\right]^{1/2} \tag{4.69}$$

where we have used the abbreviations

$$a = \left[\frac{M\omega}{\hbar f(t_b-t_a)}\right]\coth(\hbar\beta\omega)\,, \qquad b = \left[\frac{M\omega}{\hbar f(t_b-t_a)}\right]\frac{1}{\sinh(\hbar\beta\omega)}\,. \tag{4.70}$$

The symmetric and positive definite matrices $\mathbf{A}(P)$ will contain N a's along the diagonal and $(N-k)$ entries of $-b$, as well as $2k$ entries of $-b/2$, with $k\in\{0,\dots N\}$. As an example, some matrices for $N=4$ and different permutations P are given below:

$$\mathbf{A}(P_1) = \begin{pmatrix} (a-b) & 0 & 0 & 0 \\ 0 & (a-b) & 0 & 0 \\ 0 & 0 & (a-b) & 0 \\ 0 & 0 & 0 & (a-b) \end{pmatrix}, \quad \mathbf{A}(P_{10}) = \begin{pmatrix} a & -\frac{b}{2} & 0 & -\frac{b}{2} \\ -\frac{b}{2} & a & -\frac{b}{2} & 0 \\ 0 & -\frac{b}{2} & a & -\frac{b}{2} \\ -\frac{b}{2} & 0 & -\frac{b}{2} & a \end{pmatrix}, \tag{4.71}$$

$$\mathbf{A}(P_{15}) = \begin{pmatrix} a & 0 & -b & 0 \\ 0 & (a-b) & 0 & 0 \\ -b & 0 & a & 0 \\ 0 & 0 & 0 & (a-b) \end{pmatrix}, \qquad \mathbf{A}(P_{17}) = \begin{pmatrix} a & 0 & -b & 0 \\ 0 & a & 0 & -b \\ -b & 0 & a & 0 \\ 0 & -b & 0 & a \end{pmatrix}, \tag{4.72}$$

where $P_1 = \left(\begin{smallmatrix}1&2&3&4\\1&2&3&4\end{smallmatrix}\right)$ is the identity permutation and $P_{10} = \left(\begin{smallmatrix}1&2&3&4\\2&3&4&1\end{smallmatrix}\right)$, $P_{15} = \left(\begin{smallmatrix}1&2&3&4\\3&2&1&4\end{smallmatrix}\right)$, $P_{17} = \left(\begin{smallmatrix}1&2&3&4\\3&4&1&2\end{smallmatrix}\right)$. We note, that in general the matrices $\mathbf{A}(P)$ are of the following form

$$\mathbf{A}(P) = a\,\mathbb{1} - \frac{b}{2}\left[\mathbf{P}+\mathbf{P}^T\right] = a\,\mathbb{1} - \frac{b}{2}\left[\mathbf{P}+\mathbf{P}^{-1}\right]\,, \tag{4.73}$$

N	Factor per n-Cycle
1	$(a-b)$
2	$(a-b)(a+b)$
3	$(a-b)\left(a+\frac{b}{2}\right)^2$
4	$a^2(a-b)(a+b)$
5	$(a-b)\left[-a^2+-a\frac{b}{2}\left(\frac{b}{2}\right)^2\right]^2$
6	$(a-b)\left(a-\frac{b}{2}\right)^2(a+b)\left(a+\frac{b}{2}\right)^2$
7	$(a-b)\left(-a^3-a^2\frac{b}{2}+\frac{ab^2}{2}-\frac{b}{2}^3\right)^2$
8	$a^2(a-b)(a+b)\left(a^2-\frac{b^2}{2}\right)^2$
9	$(a-b)\left(a+\frac{b}{2}\right)^2\left[a^3-3a\left(\frac{b}{2}\right)^2+\left(\frac{b}{2}\right)^3\right]^2$
10	$(a-b)(a+b)\left[a^2-a\frac{b}{2}-\left(\frac{b}{2}\right)^2\right]^2\left[a^2+a\frac{b}{2}-\left(\frac{b}{2}\right)^2\right]^2$

Table 4.1: Factor in the determinant $\det(\mathbf{A}(P))$ per n-cycle in the cycle decomposition of the permutation P.

where $\mathbf{P}$ is the permutation matrix corresponding to permutation P. In the following we will show that every n-cycle in the cycle expansion of P, yields one and the same expression in the determinant of $\mathbf{A}$. This means that $\det(\mathbf{A}(P))$ has a cycle decomposition, i.e. the determinant decomposes into a product of cycle factors, each of which is a subdeterminant according to the multiplication rule for determinants $\det(AB) = \det(A)\det(B)$, and which can therefore be written as a determinant of a single-cycle matrix. Table 4.1 gives an overview of these factors up to $N = 10$.

In order to understand why $\det(\mathbf{A}(P))$ decomposes in the above way, it is useful to recall some of the properties of the symmetric group. First, we know from Section 2.1 that the group of $(N \times N)$ permutation matrices is a faithful representation of the symmetric group S_N and that the notion of conjugacy in S_N carries over to the representation group of these matrices, where it is called similarity (2.15). Thus, it follows that the representation group decomposes into similarity classes as well, i.e. into classes of permutation matrices where all matrices in the same similarity class are related by a similarity transformation (2.15). We know that similar matrices have the same determinant, so we may conjecture that our matrices (4.73) "inherit" the properties of the permutation matrices that they were constructed from. In order to verify our conjecture, we must show that they, too, obey a similarity relation which is analogous to (2.15).

In fact, this is straightforward to see: We simply apply the similarity relation for permutation matrices (2.15) to (4.73) and obtain

$$\widetilde{\mathbf{P}}^{-1}\mathbf{A}(P)\widetilde{\mathbf{P}} = a\,\mathbb{1} - \frac{b}{2}\left[\widetilde{\mathbf{P}}^{-1}\mathbf{P}\widetilde{\mathbf{P}} + \widetilde{\mathbf{P}}^{-1}\mathbf{P}^{-1}\widetilde{\mathbf{P}}\right] \tag{4.74}$$

$$= a\,\mathbb{1} - \frac{b}{2}\left[\mathbf{P}' + \mathbf{P}'^{-1}\right], \tag{4.75}$$

where $\widetilde{\mathbf{P}}$ is the respective transformation matrix for which $\widetilde{\mathbf{P}}^{-1}\mathbf{P}\widetilde{\mathbf{P}} = \mathbf{P}'$. Thus our matrices $\mathbf{A}(P)$ obey the similarity relation of the permutation matrices. This, of course, follows from the fact that they are just a linear combination of the identity matrix, a permutation matrix and its inverse.

Secondly, we observe that for every similarity class of the group of permutation matrices, there is at least one matrix $\mathbf{A}_\mathrm{D}(P_\mathrm{D})$ of the form (4.73) that is block diagonal:

$$\mathbf{A}_\mathrm{D}(P_\mathrm{D}) = \begin{pmatrix} \mathbf{B}_1 & & & \\ & \mathbf{B}_2 & & \\ & & \ddots & \\ & & & \mathbf{B}_n \end{pmatrix} , \tag{4.76}$$

where $\mathbf{B}_i$ denotes the ith sub-matrix and the empty places in (4.76) stand for sub-matrices filled with zeros. These sub-matrices may have different sizes and every one corresponds to a single cycle in the cycle decomposition of the permutation P_D, so a cycle length of d gives rise to a $d \times d$ sub-matrix in $\mathbf{A}_\mathrm{D}(P_\mathrm{D})$.

As an example, for $N = 4$, take the matrices $\mathbf{A}(P_4)$ and $\mathbf{A}(P_8)$ corresponding to permutations $P_4 = (1,3,4,2) = (1)(234)$ for the former and $P_8 = (2,1,4,3) = (12)(34)$ for the latter. Both are of block diagonal form; and as the cycle structure of their respective permutations is inequivalent, they belong to two different similarity classes:

$$\mathbf{A}(P_4) = \begin{pmatrix} (a-b) & 0 & 0 & 0 \\ 0 & a & -\frac{b}{2} & -\frac{b}{2} \\ 0 & -\frac{b}{2} & a & -\frac{b}{2} \\ 0 & -\frac{b}{2} & -\frac{b}{2} & a \end{pmatrix} , \qquad \mathbf{A}(P_8) = \begin{pmatrix} a & -b & 0 & 0 \\ -b & a & 0 & 0 \\ 0 & 0 & a & -b \\ 0 & 0 & -b & a \end{pmatrix} . \tag{4.77}$$

Now, according to our first point, any matrix (4.73) is similar to a block diagonal matrix (4.76) within the same equivalence class. Then, we can use the fact that the determinant of a block diagonal matrix is the product of determinants of the constituent sub-matrices,

$$\det \mathbf{A}_\mathrm{D}(P_\mathrm{D}) = \det(\mathbf{B}_1)\det(\mathbf{B}_2)\cdots\det(\mathbf{B}_n) , \tag{4.78}$$

yielding the explanation for the cycle decomposition of $\det(\mathbf{A}(P))$: Since every matrix $\mathbf{A}(P)$ within a certain similarity class, that is given by the cycle structure of the corresponding permutation P, is equivalent to a block diagonal matrix within the same class, they share the same determinant, which in turn, is given by the product of determinants of single-cycle sub-matrices of $\mathbf{A}(P)$.

Having explained the cycle decomposition of the determinant of the matrices (4.73), our task is now to find an explicit expression for all single-cycle subdeterminants. To simplify things, we may choose the simplest single-cycle $n \times n$ matrix, corresponding to a permutation P_{C_n} that has just one single n-cycle in its cycle decomposition. We would like to call this matrix a “modified tridiagonal matrix”, since it is a tridiagonal matrix, i.e. a matrix with only entries in the main diagonal and the first diagonal below, as well as in the first diagonal above, with two additional entries at $a_{1,n}$ and $a_{n,1}$, and denote its determinant by M_n. Note that these determinants always appear in the context of the calculation of quantities related to the harmonic oscillator in imaginary time within the path-integral formalism. The additional elements in the lower left-hand and upper right-hand corners of (4.79) are due to the periodic boundary condition $\tau = \tau + \hbar\beta$ in imaginary time [22, Chapter 2.11]. This is because the partition function is defined as the path integral over all closed cycles in imaginary time, and these two additional entries are attributed to the fact that the cycle is closed. The determinant M_n reads

$$M_n = \det\left(A_n(P)\right) = \left|\begin{array}{cccccc} a & -\frac{b}{2} & 0 & \cdots & \cdots & -\frac{b}{2} \\ -\frac{b}{2} & a & -\frac{b}{2} & 0 & \cdots & 0 \\ 0 & -\frac{b}{2} & a & -\frac{b}{2} & & \vdots \\ \vdots & 0 & -\frac{b}{2} & a & \ddots & \vdots \\ \vdots & & & \ddots & \ddots & -\frac{b}{2} \\ -\frac{b}{2} & 0 & \cdots & & -\frac{b}{2} & a \end{array}\right| \tag{4.79}$$

and corresponds to the permutation $P(C_n) = \left(\begin{smallmatrix} 1 & 2 & 3 & \dots & N-1 & N \\ 2 & 3 & 4 & \dots & N & 1 \end{smallmatrix}\right)$. Expanding it along the first row, yields a difference equation for M_n:

$$M_n = a \underbrace{\left|\begin{array}{cccccc} a & -\frac{b}{2} & 0 & \cdots & \cdots & 0 \\ -\frac{b}{2} & a & -\frac{b}{2} & 0 & \cdots & 0 \\ 0 & -\frac{b}{2} & a & -\frac{b}{2} & & \vdots \\ \vdots & 0 & -\frac{b}{2} & a & \ddots & \vdots \\ \vdots & & & \ddots & \ddots & -\frac{b}{2} \\ 0 & 0 & \cdots & & -\frac{b}{2} & a \end{array}\right|}_{T_{n-1}} - \left(-\frac{b}{2}\right) \underbrace{\left|\begin{array}{cccccc} -\frac{b}{2} & -\frac{b}{2} & 0 & \cdots & \cdots & 0 \\ 0 & a & -\frac{b}{2} & 0 & \cdots & 0 \\ 0 & -\frac{b}{2} & a & -\frac{b}{2} & & \vdots \\ \vdots & 0 & -\frac{b}{2} & a & \ddots & \vdots \\ \vdots & & & \ddots & \ddots & -\frac{b}{2} \\ -\frac{b}{2} & 0 & \cdots & & -\frac{b}{2} & a \end{array}\right|}_{C_{n-1}}$$

$$+ (-1)^{n+1}\left(-\frac{b}{2}\right) \underbrace{\left|\begin{array}{ccccccc} -\frac{b}{2} & a & -\frac{b}{2} & 0 & \cdots & & 0 \\ 0 & -\frac{b}{2} & a & -\frac{b}{2} & 0 & & \vdots \\ \vdots & 0 & -\frac{b}{2} & a & -\frac{b}{2} & 0 & \\ & & 0 & -\frac{b}{2} & a & -\frac{b}{2} & \\ & & & & \ddots & \ddots & -\frac{b}{2} \\ & & & & & & a \\ -\frac{b}{2} & 0 & \cdots & & & 0 & -\frac{b}{2} \end{array}\right|}_{D_{n-1}} . \tag{4.80}$$

The first subdeterminant in (4.80) is the determinant of a tridiagonal matrix, which we will denote in the following by T_{n-1}. It obeys the difference equation

$$T_n = aT_{n-1} - \left(\frac{b}{2}\right)^2 T_{n-2} \tag{4.81}$$

with the initial values

$$T_1 = a\ , \qquad T_2 = a^2 - (b/2)^2\ . \tag{4.82}$$

Going on, we expand the second subdeterminant – which we have named C_{n-1} – along its first row and obtain

$$C_{n-1} = \Big(-\frac{b}{2}\Big) T_{n-2} - \Big(-\frac{b}{2}\Big) \underbrace{\begin{vmatrix} 0 & -\frac{b}{2} & 0 & \cdots & \cdots & 0 \\ 0 & a & -\frac{b}{2} & 0 & & \vdots \\ 0 & -\frac{b}{2} & a & -\frac{b}{2} & 0 & \\ & 0 & -\frac{b}{2} & a & \ddots & \\ \vdots & & & \ddots & \ddots & -\frac{b}{2} \\ -\frac{b}{2} & 0 & \cdots & & -\frac{b}{2} & a \end{vmatrix}}_{\widetilde{C}_{n-2}} . \tag{4.83}$$

The resulting determinant, $\widetilde{C}_{n-2}$, reduces to $\widetilde{C}_{n-2} = (-1)^{n-1}(-b/2)\overline{C}_{n-3}$, where we find that $\overline{C}_{n-3}$ obeys the trivial recursion $\overline{C}_n = \overline{C}_{n-1}$ with the initial condition $\overline{C}_1 = (-b/2)$, which leads to $\overline{C}_n = (-b/2)^n$. Thus, the second subdeterminant gives $\widetilde{C}_{n-2} = (-1)^{n-1}(-b/2)^{n-2} = -(b/2)^{n-2}$, yielding the result

$$C_{n-1} = \Big(-\frac{b}{2}\Big) T_{n-2} + (-1)^{n-2} \Big(-\frac{b}{2}\Big)^{n-1} . \tag{4.84}$$

The third subdeterminant D_{n-1} in (4.80) is more involved. Expanding it along the first row, we obtain

$$\begin{aligned} D_{n-1} = \Big(-\frac{b}{2}\Big) & \underbrace{\begin{vmatrix} -\frac{b}{2} & a & -\frac{b}{2} & 0 & \cdots & 0 \\ 0 & -\frac{b}{2} & a & -\frac{b}{2} & & \vdots \\ \vdots & 0 & -\frac{b}{2} & a & \ddots & \vdots \\ \vdots & & 0 & -\frac{b}{2} & \ddots & -\frac{b}{2} \\ \vdots & & & \ddots & \ddots & a \\ 0 & \cdots & \cdots & \cdots & 0 & -\frac{b}{2} \end{vmatrix}}_{\overline{D}_{n-2}} - a \underbrace{\begin{vmatrix} 0 & a & -\frac{b}{2} & 0 & \cdots & 0 \\ 0 & -\frac{b}{2} & a & -\frac{b}{2} & \ddots & \vdots \\ 0 & 0 & -\frac{b}{2} & a & \ddots & 0 \\ \vdots & & 0 & -\frac{b}{2} & \ddots & -\frac{b}{2} \\ \vdots & & & \ddots & \ddots & a \\ -\frac{b}{2} & 0 & \cdots & \cdots & & -\frac{b}{2} \end{vmatrix}}_{\widetilde{D}_{n-2}} \\ + \Big(-\frac{b}{2}\Big) & \underbrace{\begin{vmatrix} 0 & -\frac{b}{2} & -\frac{b}{2} & 0 & \cdots & 0 \\ 0 & 0 & a & -\frac{b}{2} & \ddots & \vdots \\ 0 & 0 & -\frac{b}{2} & a & \ddots & 0 \\ \vdots & & 0 & -\frac{b}{2} & \ddots & -\frac{b}{2} \\ \vdots & & & \ddots & \ddots & a \\ -\frac{b}{2} & 0 & \cdots & \cdots & & -\frac{b}{2} \end{vmatrix}}_{\widetilde{\widetilde{D}}_{n-2}} , \end{aligned} \tag{4.85}$$

where again we find that $\overline{D}_{n-2}$ obeys a simple recursion since all but one of the subdeterminants in its Laplace expansion are zero, the only surviving one being $\overline{D}_{n-3}$, so we have $\overline{D}_{n-2} = (-b/2)\overline{D}_{n-3}$, with the initial condition $\overline{D}_1 = -b/2$, which yields $\overline{D}_{n-2} = (-b/2)^{n-2}$. The next term in (4.85), i.e., $\widetilde{D}_{n-2}$, may be expanded along the first column, yielding $\widetilde{D}_{n-2} =$

$(-1)^n(b/2)T_{n-3}$. Finally, the third subdeterminant $\tilde{\tilde{D}}_{N-2}$ may be expanded once along the first column, and then again along the first row, giving $\tilde{\tilde{D}}_{N-2} = (-1)^{n+1}(b^2/4)T_{n-4}$. Inserting everything into (4.80), we find that the determinant M_n for the one n-cycle matrix can be exclusively expressed in terms of only the determinant of the tridiagonal matrix T_n:

$$\begin{aligned} M_n &= aT_{n-1} + \frac{b}{2}\underbrace{\left[-\frac{b}{2}T_{n-2} - \left(\frac{b}{2}\right)^{n-1}\right]}_{C_{n-1}} \\ &\quad + (-1)^n\frac{b}{2}\underbrace{\left[\left(-\frac{b}{2}\right)^{n-1} + (-1)^{n-1}a\frac{b}{2}T_{n-3} + (-1)^n\left(\frac{b}{2}\right)^3 T_{n-4}\right]}_{D_{n-1}} \end{aligned} \tag{4.86a}$$

$$= aT_{n-1} - \frac{b^2}{4}T_{n-2} - a\frac{b^2}{4}T_{n-3} + \left(\frac{b}{2}\right)^4 T_{n-4} - 2\left(\frac{b}{2}\right)^n . \tag{4.86b}$$

Applying the difference equation (4.81) twice, even reduces (4.86b) to

$$M_n = T_n - \frac{b^2}{4}T_{n-2} - 2\left(\frac{b}{2}\right)^n . \tag{4.86c}$$

We must now find the solution to (4.81), with the initial values (4.82). Our method of preference for solving this linear difference equation with constant coefficients is the so-called Z-transform (see Appendix A), which represents a discrete Laplace-transform. Just as linear differential equations are most easily solved using Fourier or Laplace-transform, linear difference equations may be solved by employing the Z-transform. The idea contained within it was previously known as “generating function method“ and today it is used extensively in applied mathematics, digital signal processing and control theory. For our purposes, using this method has two main advantages: First, the initial values of the difference equation to be solved are automatically incorporated into the solution. Secondly, going to partial fractions in the transformed equation, yields, upon performing the inverse transformation, its solution in closed form.

We will first outline in general the method of solving a linear difference equation of order k with constant coefficients with the help of the Z-transform, and then specialise to our case of the equation for T_n. Let y_n be the original sequence and let $Y(z) = \mathcal{Z}\{y_n\}$ denote its Z-transform (A.4). Also, let the sequence g_n be given and let $G(z) = \mathcal{Z}\{g_n\}$ be its Z-transform. A general k-th order linear difference equation with constant coefficients is of the form

$$a_k y_{n+k} + a_{k-1}y_{n+k-1} + \cdots + a_2 y_{n+2} + a_1 y_{n+1} + a_0 y_n = g_n , \qquad n = 0, 1, 2, \dots , \tag{4.87}$$

where a_k are real- or complex-valued coefficients that do not depend on n, and $k \in \mathbb{R}$ denotes the number of initial conditions $y_0, y_1, \dots y_{k-1}$. By applying the second translation theorem (A.7) to (4.87), we obtain a general expression for y_n in the z-domain:

$$a_k z^k \left[Y(z) - y_0 - y_1 z^{-1} - \cdots - y_{k-1}z^{-(k-1)}\right] + \cdots + a_1 z\left[Y(z) - y_0\right] + a_0 Y(z) = G(z) . \tag{4.88}$$

With the abbreviation $p(z) = a_k z^k + a_{k-1}z^{k-1} + \cdots + a_1 z + a_0$, the solution of (4.88) in the z-domain is given by

$$Y(z) = \frac{G(z)}{p(z)} + \frac{1}{p(z)}\sum_{i=0}^{k-1} y_i \sum_{j=i+1}^{k} a_j z^{j-i} \tag{4.89}$$

and the desired result, the expression for y_n in the n-domain, either as a sequence or in closed form, is obtained, according to Section A.3, by performing the inverse Z-transform of (4.89).

In our case, keeping the notation introduced above, we have a linear, homogeneous difference equation of the form

$$y_{n+2} + a_1 y_{n+1} + a_0 y_n = 0 \ , \tag{4.90}$$

with given initial values y_1 and y_2. The second translation theorem (A.7) yields in this case

$$\mathcal{Z}\{y_{n+2}\} = z^2 \left[Y(z) - y_1 z^{-1} - y_2 z^{-2}\right] \ , \tag{4.91}$$

$$\mathcal{Z}\{y_{n+1}\} = z \left[Y(z) - y_1 z^{-1}\right] \ , \tag{4.92}$$

$$\mathcal{Z}\{y_n\} = Y(z) \tag{4.93}$$

for the three occurrences of y_i in (4.90). Inserting these into (4.90) gives us

$$z^2 \left[Y(z) - y_1 z^{-1} - y_2 z^{-2}\right] + a_1 z \left[Y(z) - y_1 z^{-1}\right] + a_0 Y(z) = 0 \ , \tag{4.94}$$

and solving for $Y(z)$ yields

$$Y(z) = \frac{(a_1 + z) y_1 + y_2}{z^2 + a_1 z + a_0} \ . \tag{4.95}$$

We now go to partial fractions of (4.95), where z_1 and z_2 are the roots of the denominator of (4.95),

$$Y(z) = \frac{(a_1 + z_1) y_1 + y_2}{(2 z_1 + a_1)(z - z_1)} + \frac{(a_1 + z_2) y_1 + y_2}{(2 z_2 + a_1)(z - z_2)} \ , \tag{4.96}$$

and may now use the identity

$$\mathcal{Z}^{-1}\left\{\frac{z}{z-a}\right\} = \mathcal{Z}^{-1}\left\{\sum_{n=0}^{\infty} \left(\frac{a}{z}\right)^n\right\} = \mathcal{Z}^{-1}\left\{\sum_{n=0}^{\infty} a^n \, z^{-n}\right\} = a^n \ , \tag{4.97}$$

which follows for instance from (A.14), the linearity of the Z-transform (A.5) yielding the relation $\mathcal{Z}^{-1}\{aY(z)\} = a y_n$, and the first translation theorem (A.6) to obtain the formula

$$\mathcal{Z}^{-1}\left\{\frac{1}{z} \frac{z}{(z - z_i)}\right\} = z_i^{n-1} \ ; \quad i = 1, 2 \tag{4.98}$$

for transforming (4.96) back to the n-domain. Thus, we obtain the following solution to (4.90) in closed form:

$$y_n = \frac{(a_1 + z_1) y_1 + y_2}{(2 z_1 + a_1)(z - z_1)} z_1^{n-1} + \frac{(a_1 + z_2) y_1 + y_2}{(2 z_2 + a_1)(z - z_2)} z_2^{n-1} \ . \tag{4.99}$$

Inserting $y_0 = T_1 = a$, $y_1 = T_2 = a^2 - (b^2/4)$ and $a_1 = a$ and $a_0 = -(b^2/4)$ yields the solution to our difference equation (4.81) for T_n:

$$T_n = \frac{1}{2^{n+1}} \left[\frac{\left(a + \sqrt{a^2 - b^2}\right)^{n+1} - \left(a - \sqrt{a^2 - b^2}\right)^{n+1}}{\sqrt{a^2 - b^2}}\right] \ . \tag{4.100}$$

We may now insert (4.100) into the difference equation (4.86c) for M_n, obtaining

$$M_n = \frac{1}{2^{n+1}} \left[\frac{\left(a + \sqrt{a^2 - b^2}\right)^{n+1} - \left(a - \sqrt{a^2 - b^2}\right)^{n+1}}{\sqrt{a^2 - b^2}} \right] - \frac{b^2}{4} \frac{1}{2^{n-1}} \left[\frac{\left(a + \sqrt{a^2 - b^2}\right)^{n-1} - \left(a - \sqrt{a^2 - b^2}\right)^{n-1}}{\sqrt{a^2 - b^2}} \right] - 2 \left(\frac{b}{2} \right)^n . \tag{4.101}$$

This can be rewritten by using $b^2 = \left(a + \sqrt{a^2 - b^2}\right)\left(a - \sqrt{a^2 - b^2}\right)$ in the second term:

$$M_n = \frac{1}{2^{n+1}} \left[\frac{\left(a + \sqrt{a^2 - b^2}\right)\left(a + \sqrt{a^2 - b^2}\right)^n - \left(a - \sqrt{a^2 - b^2}\right)\left(a - \sqrt{a^2 - b^2}\right)^n}{\sqrt{a^2 - b^2}} - \frac{\left(a - \sqrt{a^2 - b^2}\right)\left(a + \sqrt{a^2 - b^2}\right)^n - \left(a + \sqrt{a^2 - b^2}\right)\left(a - \sqrt{a^2 - b^2}\right)^n}{\sqrt{a^2 - b^2}} - 4\, b^n \right] . \tag{4.102}$$

Now, resolving the round brackets in front of every term in (4.102), six of the resulting terms cancel and we are left with

$$M_n = \frac{1}{2^{n+1}} \left[\left(a + \sqrt{a^2 - b^2}\right)^{n+1} + \left(a - \sqrt{a^2 - b^2}\right)^{n+1} - 2\, b^n \right] . \tag{4.103}$$

We may now reinsert the values of a and b, (4.70), and use the well known formulae $(\mathrm{e}^{\varphi})^n = \left(\sinh(\varphi) + \cosh(\varphi)\right)^n = \sinh(n\varphi) + \cosh(n\varphi) = \mathrm{e}^{n\varphi}$ to obtain

$$M_n = \left[\frac{M\,\omega}{\hbar\, f(t_b - t_a)} \right]^n \frac{2}{2^n \sinh^n(\hbar\beta\omega)} \left[\cosh(n\hbar\beta\omega) - 1\right] . \tag{4.104}$$

Applying the half angle formula of the hyperbolic sine gives us

$$= \left[\frac{M\,\omega}{\hbar\, f(t_b - t_a)} \right]^n \frac{1}{2^n \sinh^n(\hbar\beta\omega)} 4 \sinh^2 \left(\frac{n\hbar\beta\omega}{2} \right) , \tag{4.105}$$

which we rewrite, using the expression (3.83) for the canonical one-particle harmonic partition function $Z_1(\beta)$:

$$M_n = \left[\frac{M\,\omega}{\hbar\, f(t_b - t_a)} \right]^n \frac{1}{2^n \sinh^n(\hbar\beta\omega)} \left(\frac{1}{Z_1(n\beta)} \right)^2 . \tag{4.106}$$

Finally, we may rewrite (4.69) in cycle number notation, summing over the permutation's cycle number configuration $(C_1, \ldots, C_N)$, where C_n denotes the number of cycles with length n, and including a multiplicity factor $M(C_1, \ldots, C_N)$, as in (3.98) in Section 3.4.3, in order to be able to insert $\det A(C_N)$. We find that the factor $(2^N \sinh^N(x))^{-1}$ from above cancels the prefactors $Z_1^N(\beta)$ and $\tanh^{N/2}(\hbar\beta\omega/2)$, as well as the time-dependent one in square brackets there, so we are left with (3.100), i.e. with the well-known expression for the N-particle harmonic partition function, $Z_N(\beta)$, in cycle number notation. Thus, we have finally seen that equation (4.63) above is fulfilled, and our expression for the N-particle time-dependent density matrix is normalised, as expected.

4.7 Time Dependent Reduced One-Particle Density Matrix in *N*-Particle Ensemble

The main goal of the present section is to derive an explicit expression for the one-particle reduced density matrix $\varrho_1^{(\mathrm{r})}(x_{1b}, x_{1b'}; t_b)$ which we obtain by integrating out all of the coordinate dependencies of the N-particle density matrix except for one:

$$\varrho_1^{(\mathrm{r})}(x_{1b}, x_{1b'}; t_b) = \int_{-\infty}^{\infty} d^{N-1}x_b \; \varrho_N(x_{1b}, x_{2b}, \ldots, x_{Nb}; x_{1b'}, x_{2b}, \ldots, x_{Nb}; t_b) \, . \tag{4.107}$$

Inserting the expression for the N-particle density matrix (4.62) yields at first

$$\varrho_1^{(\mathrm{r})}(x_{1b}, x_{1b'}; t_b) = \frac{Z_1^N(\beta)}{Z_N(\beta)} \frac{1}{N!} \sum_P \epsilon^{p(P)} \times \int_{-\infty}^{\infty} d^{N-1}x_b \; \varrho_1(x_{P(1)b}, x_{1b'}; t_b) \cdots \varrho_1(x_{P(N)b}, x_{Nb}; t_b) \, . \tag{4.108}$$

We recall that the main problem with integrating out permuted coordinates of one-particle density matrices (4.18) was the presence of coordinate cross terms of the form $x_{nb}\, x_{P(n)b}$. In order to carry out these integrations, the integrals must be rearranged for every permutation, which is not feasible for the general case of N particles. Moreover, we cannot expect to integrate closed cycles by simply rearranging integrals because of the circular coordinate dependency of said cross terms. In the preceding subsection, we circumvented this problem by doing an N-dimensional Gaussian integral, at the cost of having to find an expression for the determinant of the permutation-dependent matrices $\mathbf{A}(P)$. We expect, from the insight gained previously, that the necessary $N-1$ integrations of the remaining particle coordinates are most easily done with the N-particle density matrix in some cycle reduced form, i.e. we want to integrate products of one-particle density matrices, where the coordinates are permuted according to one full cycle of the current permutation.

The additional intricacy in calculating the one-particle reduced density matrix is that now, for every permutation P, the cycle containing the remaining coordinates x_{1b} and $x_{1b'}$ is broken, a situation that we encountered before for the reduced density matrix in a two-particle ensemble, so we have to find a way to integrate arbitrary broken cycles. This fact solves the problem mentioned above, since for broken cycles the circular coordinate dependency is gone and the order of integration is straightforward, as for all coordinate cross terms within one cycle, the coordinates are now in ascending order.

Since it gives us a hint at how to proceed in this matter, we will start off by recalling the recursion relation (3.113) for the canonical partition function that was derieved in Section 3.4.3. We note that in expression (4.108) for the reduced one-particle density matrix, in every permutation, one cycle, namely the one containing the coordinates x_{1b} and $x_{1b'}$ is broken and that we arrive at an expression similar to (3.113) for the reduced one-particle density matrix, by pulling out the broken cycle of every permutation. In analogy to (3.94) in Section 3.4.3, we define the function

$$h_n^{(\mathrm{q})}(x_{1b}, x_{1b'}; \beta, t) = \int_{-\infty}^{\infty} dx_{2b} \cdots \int_{-\infty}^{\infty} dx_{nb} \; \varrho_1(x_{P(1)b}, x_{1b}; t) \times \varrho_1(x_{P(2)b}, x_{2b}; t) \cdots \varrho_1(x_{P(N)b}, x_{Nb}; t) \, , \tag{4.109}$$

for the contribution of such a broken n-cycle to the reduced density matrix, where the superscript label q indicates that it is the quenched version of (3.94). Here we see that for $t = 0$ and $x_{1b} = x_{1b'}$, we have

$$h_n^{(\mathrm{q})}(\beta) = \int_{-\infty}^{\infty} dx_{1b}\, h_n^{(\mathrm{q})}(x_{1b}, x_{1b}; \beta, t) = h_n(\beta) = Z_1(n\beta) \;, \tag{4.110}$$

which represents the corresponding contribution of a normal, i.e. a closed cycle to the canonical partition function, in accordance with (3.96). With the above considerations and definitions, we may write down the following schema for the reduced one-particle density matrix:

$$\begin{aligned} \varrho_1^{(\mathrm{r})}(x_{1b}, x_{1b'}; t_b) = \frac{Z_1^N(\beta)}{Z_N(\beta)} \frac{1}{N!} \Bigg\{ & \quad \underbrace{h_1^{(\mathrm{q})}(x_{1b}, x_{1b'}; \beta, t_b)}_{\text{Broken one-cycle}} \; Z_{N-1}(\beta) \\ & + \epsilon\, \underbrace{h_2^{(\mathrm{q})}(x_{1b}, x_{1b'}; \beta, t_b)}_{\text{Broken 2-cycle}} \; Z_{N-2}(\beta) \\ & \;\vdots \qquad\qquad\qquad\qquad\qquad \vdots \\ & + \epsilon^{N-1}\, \underbrace{h_{N-1}^{(\mathrm{q})}(x_{1b}, x_{1b'}; \beta, t_b)}_{\text{Broken } (N-1)\text{-cycle}} \; Z_1(\beta) \\ & + \epsilon^{N} \quad \underbrace{h_N^{(\mathrm{q})}(x_{1b}, x_{1b'}; \beta, t_b)}_{\text{Broken } N\text{-cycle}} \; Z_0(\beta) \Bigg\} \;. \end{aligned} \tag{4.111}$$

Now, the kth line in (4.111) corresponds to all those permutation in the sum of the original N-particle density matrix in (4.108), where the cycle that contains the coordinate x_{1b} is a k-cycle. The factor on the right in the kth line of (4.111) is then a multiple integral over all remaining closed cycles in the original permutation, each of which reduces to an n-particle partition function $Z_n(\beta)$, where $n = N - k$. When pulling out the contribution of a broken n-cycle in the above way, we must also pull out a factor of ϵ^{n+1}. This is quite easy to see: A two-cycle corresponds to a single transposition and thus comes with one single factor of ϵ. Then, a three-cycle, which corresponds to two transpositions, comes with a factor of ϵ^2, and so on. Thus, we have to pull out the above factor of ϵ^{n+1} together with every n-cycle. Writing down (4.111) in a more compact way then yields

$$\varrho_1^{(\mathrm{r})}(x_{1b}, x_{1b'}; t_b) = \frac{1}{N} \frac{1}{Z_N(\beta)} \sum_{n=1}^{N} \epsilon^{n+1} Z_1^n(\beta)\, h_n^{(\mathrm{q})}(x_{1b}, x_{1b'}; \beta, t_b)\, Z_{N-n}(\beta) \;. \tag{4.112}$$

In order to evaluate (4.112) further we must carry out the multiple integrals over broken cycles (4.109), i.e. we must integrate the product of one-particle density matrices with coordinates permuted according to a one broken-cycle permutation. We already have the right tool at hand to do this, since we obtained a master integral for integrating the broken two-cycle in Section 4.4, which is easily generalized to the case of an n-cycle. In order to see that this works, let us first calculate the master integral for a three-cycle. This is done along the same lines as in the two-particle case in equations (4.40)–(4.49), and we obtain

$$Z_1(\beta_1)Z_1(\beta_2)Z_1(\beta_3)\int_{-\infty}^{\infty}dx_{2b}\int_{-\infty}^{\infty}dx_{3b}\;\varrho_1(x_{1b},x_{2b};\beta_1,t_b)\varrho_1(x_{2b},x_{3b};\beta_2,t_b)\varrho_1(x_{3b},x_{1b'};\beta_3,t_b)$$
$$= Z_1(\beta_1+\beta_2+\beta_3)\;\varrho_1\left(x_{1b},x_{1b'};(\beta_1+\beta_2+\beta_3),t_b\right)\;. \quad (4.113)$$

Comparing (4.113) with the two-particle master integral (4.49), we see that everything is additive in β, and generalising to an n-cycle, and setting all βs equal, i.e. $\beta=\beta_1=\beta_2=\cdots=\beta_n$, yields the master integral for arbitrary broken cycles:

$$Z_1^n(\beta)\int_{-\infty}^{\infty}dx_{2b}\cdots\int_{-\infty}^{\infty}dx_{nb}\;\varrho_1(x_{1b},x_{2b};\beta,t_b)\varrho_1(x_{2b},x_{3b};t_b,\beta,t_b)\cdots\varrho_1(x_{nb},x_{1b'};\beta,t_b)$$
$$= Z_1(n\beta)\;\varrho_1(x_{1b},x_{1b'};n\beta,t_b)\;. \quad (4.114)$$

Finally, using (4.114) with (4.112) gives us the expression for the one-particle reduced density matrix in an N-particle ensemble, as the following recursion relation:

$$\varrho_1^{(\mathrm{r})}(x_{1b},x_{1b'};t_b)=\frac{1}{N}\frac{1}{Z_N(\beta)}\sum_{n=1}^{N}\epsilon^{n+1}\varrho_1(x_{1b},x_{1b'};n\beta,t_b)\;Z_1(n\beta)\;Z_{N-n}(\beta)\;. \quad (4.115)$$

In order to check that (4.115) is properly normalised, we integrate out the remaining coordinate and see, that indeed, the right-hand side evaluates to one, since the one-particle density matrix $\varrho_1(x_{1b},x_{1b'};n\beta,t_b)$ is normalised. What remains is the canonical recursion relation (3.113) for the partition function which cancels the normalisation factor $Z_N^{-1}(\beta)$.

We are now in the position to calculate the reduced one-particle width in an N-particle ensemble. It is given as the thermodynamic expectation value of x_{1b}^2, i.e. as the trace of the reduced density matrix (4.115) with the squared particle coordinate, namely

$$\sigma_1^{(\mathrm{r})2}(t_b,\beta)=\left\langle x_{1b}^2\right\rangle=\int_{-\infty}^{\infty}x_{1b}^2\;\varrho_1^{(\mathrm{r})}(x_{1b},x_{1b};\beta;t_b)\,dx_{1b}\;. \quad (4.116)$$

This is straightforward to calculate using only results from the previous sections. We obtain

$$\sigma_1^{(\mathrm{r})2}(t_b,\beta)=\frac{1}{N}\frac{1}{Z_N(\beta)}\sum_{n=1}^{N}\epsilon^{n+1}\sigma_1^2(t_b,n\beta)\;Z_1(n\beta)\;Z_{N-n}(\beta)\;, \quad (4.117)$$

where $\sigma_1^2(t_b,n\beta)$ is the time-dependent one-particle width (4.22) at an imaginary time that is scaled by the cycle length n. Pulling out the time-dependence factor $f(t_b-t_a)$, we see that, as in the one-particle case in (4.23), the reduced one-particle width (4.117) factorises into a product of the time-dependence factor above and the thermodynamic one-particle width $\sigma_1^2(\beta)$, i.e.

$$\sigma_1^{(\mathrm{r})2}(t_b,\beta)=f(t_b-t_a)\;\sigma_1^2(\beta)\;. \quad (4.118)$$

The two plots in Figure 4.4 show the thermal behaviour of (4.117) at $t=0$ for different particle numbers together with the one-particle equilibrium width $\sigma_1^2(T)$ to which (4.117) reduces for $N=1$, and for the case of bosons on the left and fermions on the right.

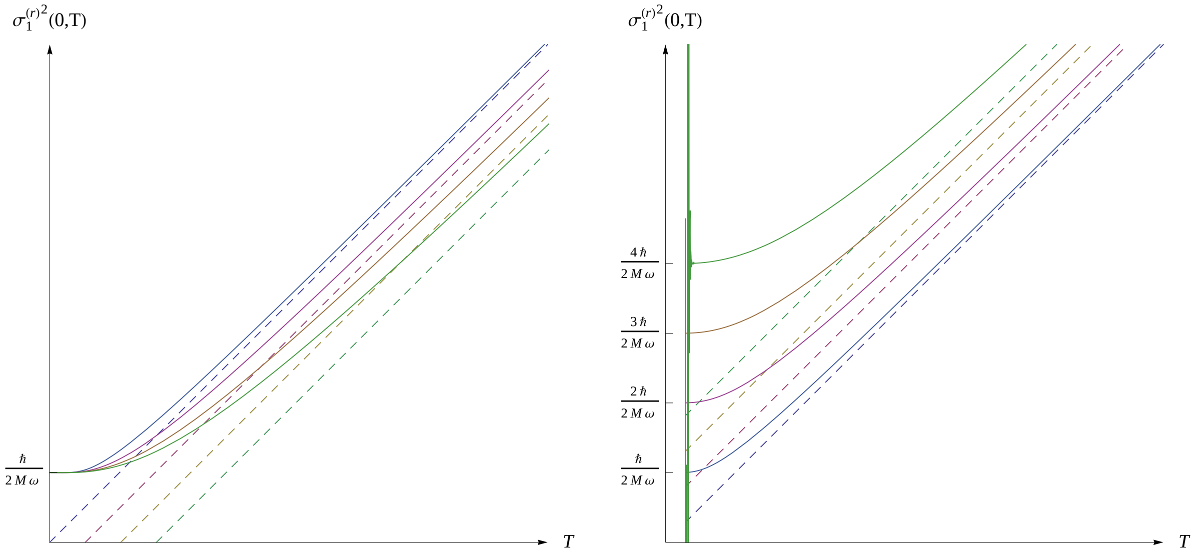

Figure 4.4: Plot of the reduced one-particle width $\sigma_1^{(\mathrm{r})2}(0,\beta)$ at $t = 0$ for bosons (left) and fermions (right) for particle numbers $N = 1$ (blue), $N = 2$ (purple), $N = 3$ (brown), and $N = 4$ (green), together with their asymptotes (4.142) (dashed), indicating the law of Dulong-Petit.

For bosons, just as in fig. 4.2, (4.117) tends to the constant value of $\hbar/(2M\omega)$ for $T \longrightarrow 0$, and approaches a linear asymptote in the high-temperature limit. At fixed temperature, the reduced one-particle width becomes smaller for increasing particle numbers, which is the expected behaviour for bosonic particles, as they can all occupy a common ground state. Note that we are assuming our system to be an ideal gas, i.e. we are treating the particles as point-like, so they do not take up any volume.

For fermions, (4.117) shows the same asymptotic behaviour, the only difference being that at fixed temperature, the reduced one-particle width is larger for increasing particle numbers. We also see, that in an N-particle ensemble, ${\sigma^{(\mathrm{r})}}^2(0,\beta)$ starts off at a ground state width that scales with N. This in turn is the behaviour that we expect from an ideal gas of fermionic particles, which is subject to the Pauli principle and thus features a non-zero degeneracy pressure even at $T = 0$.

Note that the curves in the right plot of Fig. 4.4 oscillate strongly for low temperatures. This seems to be a numerical problem, i.e. an artefact of finite numerical resolution which indicates that a different numerical approach is necessary in the fermionic case. Here, we include the fermionic plot for the sake of completeness. The above curves were obtained by directly programming the recursions (3.113) and (4.117) in Mathematica, which worked reasonably well only for very small particle numbers up to approximately $N = 6$.

For both plots in Fig. 4.2, the linear asymptotes for different particle numbers seem to have the same slope, but different y-intercepts and we naturally expect the y-intercepts of the graph of (4.117) to depend on the particle number N. The difference between bosonic and fermionic gases seems to manifest itself in the sign, where the asymptotes for bosons have negative and the asymptotes for fermions positive y-intercepts.

In the following, we will derive the expression for these high-temperature asymptotes. Looking at equation (4.117), it is clear that we need to know the asymptotic behaviour of the N-particle partition function in order to evaluate the reduced one-particle width in this limit. To that end, let us recall the canonical partition function in cycle reduced form (3.98), and, for a start, let us take the simplest term in the sum of (3.98), namely the one where $n = 1$, $C_1 = N$, and $C_n = 0$ for $n > 1$, for a permutation that consists only of one-cycles. In the limit $T \to \infty$ we may expand the hyperbolic sine in the expression for $Z_1(\beta)$ in equation (3.83) and neglect all higher order terms in T, obtaining

$$Z_1(\beta) \xrightarrow{T\to\infty} \left(\frac{M\omega}{\hbar}\right)\left(\frac{k_{\mathrm{B}}T}{M\omega^2}\right) . \tag{4.119}$$

Using this with (3.98) for the simple permutation above, we see that it contributes a term that is proportional to $(\frac{M\omega}{\hbar})^N(\frac{k_{\mathrm{B}}T}{M\omega^2})^N$ to $Z_N(\beta)$. In fact, because of the condition $\sum_n C_n n = N$ that is imposed on the sum over cycle configurations in (3.98), the product over all cycle numbers of $[Z_1(n\beta)]^{C_n}$ yields the same asymptotic contribution to $Z_N(\beta)$ (up to a factor) for *every* permutation. Thus, we have found that asymptotically, i.e. for $T \to \infty$, $\beta \to 0$ and to leading order in T, the N-particle partition function is given by

$$Z_N(\beta) = \frac{1}{N!}\, Z_1^N(\beta) = \frac{1}{N!}\left(\frac{M\omega}{\hbar}\right)^N\left(\frac{k_{\mathrm{B}}T}{M\omega^2}\right)^N . \tag{4.120}$$

We are also interested in the next-to-leading order of the asymptotic expression for $Z_N(\beta)$, since we expect its prefactor to be important for the y-intercepts of the linear asymptotes of (4.117). Thus, our ansatz for $Z_N(\beta)$ is:

$$Z_N(\beta) \approx \frac{1}{N!}\left(\frac{M\omega}{\hbar}\right)^N\left(\frac{k_{\mathrm{B}}T}{M\omega^2}\right)^N + A_N\left(\frac{M\omega}{\hbar}\right)^{N-1}\left(\frac{k_{\mathrm{B}}T}{M\omega^2}\right)^{N-1} . \tag{4.121}$$

We plan to insert this expression into the recursion relation for (3.113) $Z_N(\beta)$, and by comparing coefficients, obtain a corresponding recursion for A_N. Solving this recursion and using our ansatz (4.121) with the time-independent version of (4.117) should then yield the prefactor mentioned above. Putting (4.121) into (3.113) we get

$$\begin{aligned}
&\frac{1}{N!}\left(\frac{M\omega}{\hbar}\right)^N\left(\frac{k_{\mathrm{B}}T}{M\omega^2}\right)^N + A_N\left(\frac{M\omega}{\hbar}\right)^{N-1}\left(\frac{k_{\mathrm{B}}T}{M\omega^2}\right)^{N-1}\\
&= \frac{1}{N}\sum_{n=1}^{N}\left[\frac{1}{n}\frac{\epsilon^{n+1}}{(N-n)!}\left(\frac{M\omega}{\hbar}\right)^{N-n+1}\left(\frac{k_{\mathrm{B}}T}{M\omega^2}\right)^{N-n+1} + \epsilon^{n+1}\frac{A_{N-n}}{n}\left(\frac{M\omega}{\hbar}\right)^{N-n}\left(\frac{k_{\mathrm{B}}T}{M\omega^2}\right)^{N-n}\right] ,
\end{aligned} \tag{4.122}$$

and comparing powers of T on both sides, it is clear that on the right-hand side of (4.122) the first term contributes only for $n = 1$ and $n = 2$, and the second term only for $n = 1$. Thus we obtain

$$\begin{aligned}
&\frac{1}{N!}\left(\frac{M\omega}{\hbar}\right)^N\left(\frac{k_{\mathrm{B}}T}{M\omega^2}\right)^N + A_N\left(\frac{M\omega}{\hbar}\right)^{N-1}\left(\frac{k_{\mathrm{B}}T}{M\omega^2}\right)^{N-1}\\
&\qquad = \frac{\epsilon^2}{N!}\left(\frac{M\omega}{\hbar}\right)^N\left(\frac{k_{\mathrm{B}}T}{M\omega^2}\right)^N + \frac{\epsilon^3}{2}\frac{(N-1)}{N!}\left(\frac{M\omega}{\hbar}\right)^{N-1}\left(\frac{k_{\mathrm{B}}T}{M\omega^2}\right)^{N-1}\\
&\qquad\qquad + \epsilon^2\frac{A_{N-1}}{N}\left(\frac{M\omega}{\hbar}\right)^{N-1}\left(\frac{k_{\mathrm{B}}T}{M\omega^2}\right)^{N-1} ,
\end{aligned} \tag{4.123}$$

which reduces to the following recursion for A_N:

$$A_N - \frac{A_{N-1}}{N} = \pm\frac{1}{2}\frac{(N-1)}{N!} \;, \tag{4.124}$$

where the plus sign of the right-hand side of (4.124) is for bosons and the minus sign for fermions. The initial condition for A_N must be $A_0 = A_1 = 0$, in order for our ansatz (4.121) to be consistent with the values of $Z_0(\beta) = 1$ and the asymptote (4.119) for $Z_1(\beta)$. The recursion above may be solved by employing the *generating function method*, which can be thought of as the precursor of the Z-Transform from Appendix A. The idea contained within this method is to extend the given recursion to a formal power series, whose coefficients are those of the recursion, thus "transforming" it into a holomorphic function.

First, for typographical and aesthetic reasons, we rename N to n. Now we will define the generating function of A_n to be

$$f(z) = \sum_{n=1}^{\infty} A_n z^n \;. \tag{4.125}$$

Multiplying (4.124) with z^n and formally summing from $n = 1$ to $n = \infty$ yields

$$\sum_{n=1}^{\infty} A_n z^n - \sum_{n=1}^{\infty} \frac{A_{n-1}}{n} z^n = \pm\frac{1}{2}\sum_{n=1}^{\infty}\frac{(n-1)}{n!} z^n \;. \tag{4.126}$$

We this rewrite in the following form, using an integration in the second sum of (4.126) to get rid of the factor $1/n$ there:

$$f(z) - \sum_{n=1}^{\infty} A_{n-1} \int_0^z z'^{n-1}\, dz' = \pm\frac{1}{2}\left[z\sum_{n=1}^{\infty}\frac{z^{n-1}}{(n-1)!} - \sum_{n=1}^{\infty}\frac{z^n}{n!}\right] \;. \tag{4.127}$$

We swap sum and integral in the second term on the left-hand side of (4.127), and pull out the term with $n = 0$ from the sum, noting that it vanishes because of the initial condition $A_0 = A_1 = 0$. In the first sum on the right-hand side we adjust the summation index and in the last sum we may add and subtract one, to turn both sums into exponentials:

$$f(z) - \int_0^z \left(A_0 z'^0 + \sum_{n=1}^{\infty} A_n z'^n \right) dz' = \pm\frac{1}{2}\left[z\sum_{n=0}^{\infty}\frac{z^n}{n!} - \left(\sum_{n=0}^{\infty}\frac{z^n}{n!} - 1\right)\right] \;. \tag{4.128}$$

Thus we are left with an integral equation for $f(z)$

$$f(z) - \int_0^z f(z')\, dz' = \pm\frac{1}{2}\Big[z\mathrm{e}^z - \mathrm{e}^z + 1\Big] \;. \tag{4.129}$$

Differentiating (4.129) removes the integral and yields a linear inhomogeneous first-order constant coefficient differential equation for $f(z)$ with:

$$f'(z) - f(z) = \pm\frac{1}{2}\, z\, \mathrm{e}^z \;. \tag{4.130}$$

This may be solved by the *method of variation of parameters*.

Such an inhomogeneous first-order linear differential equation with constant coefficients is of the form

$$y'(z) + p\, y(z) = q(z) \tag{4.131}$$

and has the general solution in terms of a constant c and a variable parameter $c(z)$

$$y(z) = c\, \mathrm{e}^{-pz} + c(z)\, \mathrm{e}^{-pz} \,, \tag{4.132}$$

where $c = y(z_0)$ and $c(z) = \int_{z_0}^{z} q(z')\, \mathrm{e}^{pz'}\, dz'$. In our case, we have $p = -1$, $q(z) = \pm\frac{1}{2}\, z\, \mathrm{e}^{z}$ and because of $A_1 = 0$ and the initial condition $f(0) = 0$, the general solution of (4.130) consists only of the second term of (4.132). It is

$$f(z) = \pm\frac{1}{4}\, z^2\, \mathrm{e}^{z} \,. \tag{4.133}$$

Now, transforming (4.133) back to the n-domain is straightforward: We must rewrite every term as a sum $\sum_{n=1}^{\infty} c_n z^n$ and simply read off the coefficients c_n:

$$\sum_{n=1}^{\infty} A_n z^n = \pm\frac{1}{4}\, z^2 \sum_{n=0}^{\infty} \frac{z^n}{n!} = \pm\frac{1}{4}\Big[\frac{z^2}{0!} + \frac{z^3}{1!} + \frac{z^4}{2!} + \cdots\Big] \tag{4.134}$$

and because of $1/(-1)! = 0$ we may rewrite the right-hand side of (4.134) as

$$\sum_{n=1}^{\infty} A_n z^n = \pm\frac{1}{4}\Big[\frac{z^1}{(-1)!} + \frac{z^2}{0!} + \frac{z^3}{1!} + \frac{z^4}{2!} + \cdots\Big] = \pm\sum_{n=1}^{\infty} \frac{1}{4}\frac{z^n}{(n-2)!} \,, \tag{4.135}$$

to obtain

$$A_N = \pm\frac{1}{4}\frac{1}{(N-2)!} \,, \tag{4.136}$$

where we have renamed the index variable n back to N again.

We are now in the position to insert our ansatz (4.121) for $Z_N(\beta)$ into the recursion relation (4.117) for the reduced one-particle width. Using

$$Z_1(n\,\beta) \approx \frac{1}{n}\left(\frac{M\omega}{\hbar}\right)\left(\frac{k_{\mathrm{B}}T}{M\omega^2}\right) \,, \qquad \sigma_1^2(n\,\beta) \approx \frac{1}{n}\left(\frac{k_{\mathrm{B}}T}{M\omega^2}\right) \tag{4.137}$$

we have

$$\begin{aligned}
\sigma_1^{(\mathrm{r})2}(\beta) \approx{}& \frac{\left(\frac{k_{\mathrm{B}}T}{M\omega^2}\right)\left(\frac{M\omega}{\hbar}\right)\left(\frac{k_{\mathrm{B}}T}{M\omega^2}\right)\left[\frac{1}{(N-1)!}\left(\frac{M\omega}{\hbar}\frac{k_{\mathrm{B}}T}{M\omega^2}\right)^{N-1} \pm \frac{(N-1)(N-2)}{4(N-1)!}\left(\frac{M\omega}{\hbar}\frac{k_{\mathrm{B}}T}{M\omega^2}\right)^{N-2}\right]}{N\left[\frac{1}{N!}\left(\frac{M\omega}{\hbar}\frac{k_{\mathrm{B}}T}{M\omega^2}\right)^{N} \pm \frac{N(N-1)}{4N!}\left(\frac{M\omega}{\hbar}\frac{k_{\mathrm{B}}T}{M\omega^2}\right)^{N-1}\right]} \\
&+ \frac{\frac{1}{2}\left(\frac{k_{\mathrm{B}}T}{M\omega^2}\right)\frac{1}{2}\left(\frac{M\omega}{\hbar}\right)\left(\frac{k_{\mathrm{B}}T}{M\omega^2}\right)\frac{1}{(N-2)!}\left(\frac{M\omega}{\hbar}\frac{k_{\mathrm{B}}T}{M\omega^2}\right)^{N-2}}{N\left[\frac{1}{N!}\left(\frac{M\omega}{\hbar}\frac{k_{\mathrm{B}}T}{M\omega^2}\right)^{N} \pm \frac{N(N-1)}{4N!}\left(\frac{M\omega}{\hbar}\frac{k_{\mathrm{B}}T}{M\omega^2}\right)^{N-1}\right]} \,.
\end{aligned} \tag{4.138}$$

In a first step, we may pull out equal factors of $\frac{1}{(N-1)!}(\frac{M\omega}{\hbar})^{N-1}(\frac{k_\mathrm{B}T}{M\omega^2})^{N-1}$ from the numerator and denominator on the right-hand side of (4.138), which cancel. What remains is

$$\sigma_1^{(\mathrm{r})2}(\beta) \approx \frac{\left(\frac{M\omega}{\hbar}\right)\left(\frac{k_\mathrm{B}T}{M\omega^2}\right)^2 \pm \frac{(N-1)(N-2)\pm(N-1)}{4}\left(\frac{k_\mathrm{B}T}{M\omega^2}\right)}{\left[\left(\frac{M\omega}{\hbar}\right)\left(\frac{k_\mathrm{B}T}{M\omega^2}\right) \pm \frac{N(N-1)}{4}\right]} \, . \tag{4.139}$$

A polynomial long division of the right-hand side of (4.139) yields

$$\frac{ax^2 \pm \frac{(N-1)^2 x}{4}}{ax \pm \frac{N(N-1)}{4}} = x \mp \frac{(N-1)}{4a} + O(x^{-1}) \tag{4.140}$$

with the abbreviations

$$a = \frac{M\omega}{\hbar} \, , \qquad x = \frac{k_\mathrm{B}T}{M\omega^2} \, . \tag{4.141}$$

Using this result, we obtain the following expression for the asymptotic behaviour of the reduced one-particle width:

$$\sigma_1^{(\mathrm{r})2}(\beta) \xrightarrow{T\to\infty} \left(\frac{k_\mathrm{B}T}{M\omega^2}\right) \mp \frac{(N-1)}{4}\left(\frac{\hbar}{M\omega}\right) \, , \tag{4.142}$$

where again, the upper sign is for bosons and the lower sign is for fermions.

4.8 Comparison with Grand Canonical Ensemble

In the grand canonical ensemble, the grand canonical density operator is given by (3.10) with the Hamiltonian in coordinate representation $\hat{H} = \hat{H}_\omega = -\frac{\hbar^2}{2M}\frac{d^2}{dx^2} + \frac{M}{2}\omega^2 x^2$ where ω is the equilibrium trap frequency. A quench in trap frequency (4.2) is then described by the time evolution with the harmonic oscillator Hamiltonian (4.8) with trap frequency Ω, i.e.

$$\hat{\varrho}_\mathrm{GK}(t_b) = \frac{1}{\mathcal{Z}(\beta)} \mathrm{e}^{-\frac{i}{\hbar}\hat{H}_\Omega(t_b-t_a)} \mathrm{e}^{-\beta(\hat{H}_\omega-\mu\hat{N}} \mathrm{e}^{\frac{i}{\hbar}\hat{H}_\Omega(t_b-t_a)} \, . \tag{4.143}$$

Now, going to the coordinate base matrix representation by sandwiching (4.143) between position eigenstates is not as straightforward as in (4.7), since in the grand canonical ensemble the particle number is not fixed but left free to fluctuate. Consequently, we must use multiparticle states with a variable or unknown number of particles and these are precisely the continuous Fock space position eigenstates (2.82) that were introduced in Section 2.3.1. Now, sandwiching the time-dependent density operator (4.143) between these multi-particle states (2.82) yields

$$\begin{aligned} &\varrho_\mathrm{GK}(x_{1b},\dots;x_{1b'},\dots;\beta,t_b) = \\ &\frac{1}{\mathcal{Z}(\beta)} \sum_{N=1}^{\infty}\sum_{N'=1}^{\infty} {}^{(\epsilon)}\langle N; x_{1b},\dots,x_{Nb}|\, \mathrm{e}^{-\frac{i}{\hbar}\hat{H}_\Omega(t_b-t_a)} \mathrm{e}^{-\beta(\hat{H}_\omega-\mu\hat{N})} \mathrm{e}^{\frac{i}{\hbar}\hat{H}_\Omega(t_b-t_a)} \, |N'; x_{1b'},\dots,x_{Nb'}\rangle^{(\epsilon)} \, . \end{aligned} \tag{4.144}$$

As, according to (2.53), two many-particle states (2.79) in (2.82) with different particle numbers N and N' are orthogonal, and as there are no operators in the two Hamiltonians in (4.143) that change particle numbers, the two sums in (4.144) reduce to one. We may now insert the

Fock space completeness relation (2.80) twice, between time evolution operator and density operator in (4.144), once with $x_{1a}, \dots$ and once with $x_{1a'}, \dots$ to obtain

$$
\begin{aligned}
&\varrho_{\mathrm{GK}}(x_{1b}, \dots; x_{1b'}, \dots; \beta, t_b) = \\
&\frac{1}{\mathcal{Z}(\beta)} \sum_{N=1}^{\infty} \int dx_{1a} \cdots dx_{Na} \int dx_{1a'} \cdots dx_{Na'} \, {}^{(\epsilon)}\langle N; x_{1b}, \dots, x_{Nb} | \, \mathrm{e}^{-\frac{i}{\hbar} \hat{H}_{\Omega}(t_b - t_a)} \, | N; x_{1a}, \dots, x_{Na} \rangle^{(\epsilon)} \\
&\qquad\qquad {}^{(\epsilon)}\langle N; x_{1a}, \dots, x_{Na} | \, \mathrm{e}^{-\beta(\hat{H}_{\omega} - \mu \hat{N})} \, | N; x_{1a'}, \dots, x_{Na'} \rangle^{(\epsilon)} \\
&\qquad\qquad\qquad {}^{(\epsilon)}\langle N; x_{1a'}, \dots, x_{Na'} | \, \mathrm{e}^{\frac{i}{\hbar} \hat{H}_{\Omega}(t_b - t_a)} \, | N'; x_{1b}, \dots, x_{Nb} \rangle^{(\epsilon)} \, . \qquad (4.145)
\end{aligned}
$$

In the centre amplitude in (4.145), we may factorise the operator exponential $\exp\{-\beta(\hat{H}_\omega - \mu \hat{N})\}$, since $\hat{H}_\omega$ and $\hat{N}$ commute and let $\exp\{\beta\mu\hat{N}\}$ act on the state to the right. We see that the remaining three amplitudes are the same ones as in our ansatz for the canonical N-particle time-dependent density matrix (4.52). The only differences between the canonical ansatz (4.52) and the grand canonical analogue in (4.145) are, that in the latter the normalisation factor is the inverse of the grand canonical partition function $\mathcal{Z}(\beta)$, instead of the canonical one, and that in (4.145) we have a sum of (4.52) over all possible particle numbers, weighted with $\exp\{-\beta\mu N\}$, which is the unnormalised probability for a state with particle number N to occur. Thus, the time-dependent grand canonical density matrix reads:

$$
\varrho_{\mathrm{GK}}(x_{1b}, \dots; x_{1b'}, \dots; \beta, t_b) = \frac{1}{\mathcal{Z}(\beta)} \sum_{N=1}^{\infty} \mathrm{e}^{\beta\mu N} \, \varrho_N(x_{1b}, \dots, x_{Nb}; x_{1b'}, \dots, x_{Nb'}; t_b) \, Z_N(\beta) \, . \tag{4.146}
$$

Setting $x_{nb} = x_{nb'}$ for all n and subsequently integrating out all coordinates in (4.146) should then yield the grand canonical partition function, however, there remains the question of how to define this integration on the states (2.82). A sensible choice is to take the infinite direct sum of tensor products between integral operators over x_{nb} for all n, that is to define the integration operator

$$
\hat{I} = \int_{-\infty}^{\infty} dx_{1b} \, \oplus \, \left(\int_{-\infty}^{\infty} dx_{1b} \int_{-\infty}^{\infty} dx_{2b} \right) \oplus \left(\int_{-\infty}^{\infty} dx_{1b} \int_{-\infty}^{\infty} dx_{2b} \int_{-\infty}^{\infty} dx_{3b} \right) \oplus \cdots \, . \tag{4.147}
$$

Applying $\hat{I}$ to (4.146) then yields the well-known expression (3.101) for the grand canonical partition function in terms of canonical partition functions:

$$
\mathcal{Z}(\beta) = \sum_{N=0}^{\infty} Z_N(\beta) \, \mathrm{e}^{\beta\mu N} \, . \tag{4.148}
$$

Equally, we obtain an expression for the reduced grand canonical time-dependent density matrix by applying to (4.146) an integration operator, that acts on the coordinates $x_{2b}, \dots$ and leaves out $x_{1b}, x_{1b'}$ from integration. In analogy to (4.147), we define the *reduced* integration operator

$$
\hat{I}^{(\mathrm{r})} = \mathbb{1} \oplus \int_{-\infty}^{\infty} dx_{2b} \oplus \left(\int_{-\infty}^{\infty} dx_{2b} \int_{-\infty}^{\infty} dx_{3b} \right) \oplus \left(\int_{-\infty}^{\infty} dx_{2b} \int_{-\infty}^{\infty} dx_{3b} \int_{-\infty}^{\infty} dx_{4b} \right) \oplus \cdots \, , \tag{4.149}
$$

so that applying $\hat{I}^{(\mathrm{r})}$ to (4.146) yields

$$\varrho^{(\mathrm{r})}_{\mathrm{GK}}(x_{1b}, x_{1b'}; \beta, t_b) = \frac{1}{\mathcal{Z}(\beta)} \sum_{N=1}^{\infty} \mathrm{e}^{\beta\mu N} \; \varrho^{(\mathrm{r})}_{1,N}(x_{1b}, x_{1b'}; t_b) \; Z_N(\beta) \; . \tag{4.150}$$

Here we have given the reduced canonical density matrix in (4.150) an extra index N, to indicate that it is the reduced canonical density matrix in an N-particle ensemble. We may simplify (4.150) further by inserting the right side of (4.115) for the reduced canonical density matrix, where we find that the canonical partition function $Z_N(\beta)$ there cancels and we are left with

$$\varrho^{(\mathrm{r})}_{\mathrm{GK}}(x_{1b}, x_{1b'}; \beta, t_b) = \frac{1}{\mathcal{Z}(\beta)} \sum_{N=1}^{\infty} \frac{\mathrm{e}^{\beta\mu N}}{N} \sum_{k=1}^{N} \epsilon^{k+1} \varrho_1(x_{1b}, x_{1b'}; k\beta, t_b) \; Z_1(k\beta) \; Z_{N-k}(\beta) \; . \tag{4.151}$$

In order to compare our result (4.151) to grand-canonical expressions we note, that we have calculated the density matrix, i.e. the quantum mechanical expectation value for the frequency-quenched density operator (4.143), which is normalised to unity. In contrast, the reduced grand-canonical one-particle particle density is normalised to the particle number N, as we will see in the following.

For an introduction to the grand-canonical description of local quantities, such as density matrices and propagators, see, e.g. [29, Section 2.3], and for a more complete treatment we refer the reader to the thesis [30, Chapter 2]. The single-particle imaginary-time grand-canonical propagator $G(x_1, \tau_1; x_2, \tau_2)$, which is here taken to be in one dimension, represents the probability for a single particle created at point x_2 in imaginary time τ_2 to go to point x_1 at imaginary time τ_1, where it is annihilated. It is given as the thermal expectation value of the time-ordered product $\hat{T}\left[\hat{a}(x_1, \tau_1)\hat{a}^{\dagger}(x_2, \tau_2)\right]$ of the annihilation and creation operators, i.e. as the trace

$$G(x_1, \tau_1; x_2, \tau_2) = \mathrm{Tr}\left\{\hat{\varrho}_{\mathrm{GK}} \, \hat{T}\left[\hat{a}(x_1, \tau_1)\hat{a}^{\dagger}(x_2, \tau_2)\right]\right\} . \tag{4.152}$$

For bosons, the above expression (4.152) may be evaluated via its spectral representation in Matsubara space. The lengthy calculation yields

$$G(x_1, \tau_1; x_2, \tau_2) = \sum_{n=-\infty}^{\infty} \Theta(\tau_2 - \tau_1 + n\hbar\beta) \; (x_2, \tau_2 - \tau_1 + n\hbar\beta \mid x_1, \; 0)\Big|_{E_k \to E_k - \mu} , \tag{4.153}$$

so the grand-canonical propagator is given in terms of an imaginary-time evolution amplitude (3.17). From this we obtain the corresponding bosonic grand-canonical particle density at point x_1 by taking the diagonal elements of (4.153) in the limit $\tau_2 \nearrow \tau_1$, which leaves us with

$$n_{\mathrm{GK}}(x_1, \beta) = \lim_{\tau_2 \nearrow \tau_1} G(x_1, \tau_1; x_2, \tau_2) = \sum_{n=1}^{\infty} (x_1, n\hbar\beta \mid x_1, 0) \, \mathrm{e}^{n\beta\mu} \; . \tag{4.154}$$

We obtain the time-dependent canonical version of (4.154) by multiplying our result for the canonical one-particle density matrix by N:

$$n(x_{1b}, \beta, t_b) = N \, \varrho_{1,N}(x_{1b}, x_{1b}; \beta, t_b) \; . \tag{4.155}$$

Inserting (4.155) into (4.151) cancels the factor $1/N$ and yields the time-dependent grand-canonical particle density

$$n_{\mathrm{GK}}(x_{1b},\beta,t_b) = \frac{1}{\mathcal{Z}(\beta)} \sum_{N=1}^{\infty} \mathrm{e}^{\beta\mu N} \sum_{k=1}^{N} \epsilon^{k+1} \varrho_1(x_{1b},x_{1b};k\beta,t_b)\, Z_1(k\beta)\, Z_{N-k}(\beta)\ . \tag{4.156}$$

The two sums in (4.156) are a Cauchy product of the form $\sum_{n=0}^{\infty}\sum_{k=0}^{n} a_k b_{n-k} = (\sum_{n=0}^{\infty} a_n)(\sum_{k=0}^{\infty} b_k)$ and by setting $N' = N-k$ we obtain

$$n_{\mathrm{GK}}(x_{1b},\beta,t_b) = \frac{1}{\mathcal{Z}(\beta)} \left(\sum_{N'=1}^{\infty} \mathrm{e}^{\beta\mu N'} Z_{N'}(\beta) \right) \sum_{k=1}^{\infty} \epsilon^{k+1}\, \mathrm{e}^{\beta\mu k}\, \varrho_1(x_{1b},x_{1b};k\beta,t_b)\, Z_1(k\beta)\ , \tag{4.157}$$

where in the first sum in round braces we recognise the expression for the grand canonical partition function (4.148). Thus, we are left with

$$n_{\mathrm{GK}}(x_{1b},\beta,t_b) = \sum_{n=1}^{\infty} \epsilon^{n+1}\, \mathrm{e}^{\beta\mu n}\, \varrho_1(x_{1b},x_{1b};n\beta,t_b)\, Z_1(n\beta)\ , \tag{4.158}$$

which reduces to the above expression (4.154) for the grand canonical density by taking (4.158) at $t=0$ and using (4.18) and (4.56) to write the combination of canonical one-particle density matrix and canonical one-particle partition function above as a one-particle imaginary time amplitude:

$$n_{\mathrm{GK}}(x_{1b},\beta) = \sum_{n=1}^{\infty} \epsilon^{n+1}\ (x_{1b}, n\beta \mid x_{1b}, 0)\ \mathrm{e}^{n\beta\mu}\ , \tag{4.159}$$

where our result is valid both for bosons and fermions.

Chapter 5

Summary

In this thesis, we investigated the effect of a quench, i.e. of a sudden change, of trap frequency on harmonically trapped ideal quantum gases in the canonical ensemble.

The introductory Chapter 1 was devoted to ideal quantum gases in equilibrium and non-equilibrium situations. Here, we first gave a short historical introduction to Bose-Einstein condensation, presenting a simple argument for the occurrence of this purely quantum statistical phase transition. We then briefly reviewed the experimental challenges of BEC research, e.g. the metastability of the BEC regime and the techniques of both laser cooling and evaporative cooling that finally led to the realisation of the first condensates in 1995.

We then passed on to non-equilibrium phenomena in Section 1.2, noting, that the notion of equilibrium state is only an approximation and that in reality, all systems are constantly in a non-equilibrium state. We mentioned two general classes of experimental situations and their mathematical description. The first is perturbation theory, where the Hamiltonian of the system can be split into a time-independent and a perturbation part, and the second is that of a quench, i.e. a sudden change in a parameter of the Hamiltonian. As an experimental motivation, then gave two important examples of the latter in the following two subsections: time-of-flight imaging, where the trapping potential is quenched to zero and where subsequently images of the expanding atomic cloud are taken, and secondly the observation of collapse and revival of the coherent matter-wave interference pattern in optical lattices, following a quench of the optical lattice potential. At the end of Chapter 1, we then presented a short overview of this thesis.

In Chapter 2, we laid the foundations for the canonical description of ideal quantum gases. We began by introducing permutations and the symmetric group in Section 2.1, as well as permutation matrices, which are faithful representations of the symmetric group. We then defined the notion of permutation cycles, the importance of which lie in the fact that every permutation has a unique decomposition in terms of cycles, i.e. a unique cycle structure. We introduced the equivalence relation of conjugacy in the symmetric group, which partitions it into conjugacy classes, where the conjugacy classes correspond to the cycle structure of group members. We found that the notion of conjugacy carries over to the representation group of permutation matrices, where it is called similarity. In Section 2.2 we then reviewed the quantum mechanics of a many-particle system, introducing the notion of distinguishable and identical particles. From the defining equation for the states of systems of identical particles (2.20), we found that these states must be invariant under the action of the symmetric group in the form of the permutation operator (2.37), which therefore commutes with every observable of the system. We then introduced the continuous and the discrete Hilbert space of (anti-)symmetrised particles and the Fock space of variable particle numbers.

Chapter 3 then deals with the canonical and grand-canonical description of ideal quantum gases. In Section 3.1 we first gave a brief introduction to statistical mechanics, introducing the micro-canonical, canonical, and grand-canonical ensembles. In the following sections, we then introduced the one-particle time evolution amplitude as the expectation value of the time-evolution operator and its properties, as well as the notion of Wick rotation. We then turned to the path integral representation of quantum mechanics, motivating the Van-Vleck-Pauli-Morette formula (3.55), which we use to derive the one dimensional time evolution amplitude of the harmonic oscillator and the single-particle, one-dimensional density matrix in imaginary time (3.82), as well as the explicit expression for the one-particle partition function (3.83). From this we calculated the many-particle partition function in cycle reduced form (3.100), and in the form of a recursion (3.113).

In Chapter 4 we presented our own main results. Starting with the single-particle density operator of the harmonic oscillator in *imaginary time* (3.82), we calculated the time-evolution with the *real time* Hamiltonian of the harmonic oscillator (4.8), thus separating the equilibrium dynamics from the non-equilibrium dynamics in parameter space. After taking the expectation value in coordinate representation and by inserting corresponding completeness relations between the initial density operator and the time-evolution operators, we obtained the time-dependent one-particle density matrix as the normalised product (4.10) of three time-evolution amplitudes. The subsequent integration (4.15) then yielded the explicit expression (4.18) for the time-dependent one-particle density matrix. This was found to have the same form as the equilibrium density matrix (3.82) up to the function (4.19), which appears in the prefactor and in the exponential of (4.18) and which carries the time-dependence. The time-dependent oscillator width (4.22) was found to factorise into the well-known thermodynamic width, which we display in Fig. 4.2, and the above time-dependence function. For a quench at time $t = 0$, this function can be brought into the form (4.24), where the two-fold final frequency Ω appears in the argument of a cosine. Its oscillatory behaviour is depicted in the two plots of Fig. 4.3. Thus, the time-dependent single-particle width oscillates in time with twice the frequency of the final harmonic potential without damping.

In Section 4.2, we extended our discussion to the case of a two-particle system. We used the same ansatz as for the one-particle case, except that the density matrix (4.25) now consisted of many-particle time-evolution amplitudes (4.26)–(4.28) in terms of the two different permutations (12) and (21). By rearranging the one-particle amplitudes and using the relation (4.31), we obtained the expression (4.32) for the two-particle time-dependent density matrix in terms of one-particle ones. In Section 4.3 we then verified that the two-particle partition function follows from the continuous trace of (4.32), and in Section 4.4 we calculated the reduced one-particle density matrix in a two-particle ensemble (4.50) by performing a partial trace of (4.32), as well as the time-dependent two-particle width (4.51)

In Section 4.5, the above steps were repeated for the general case of an N-particle ensemble. The ansatz (4.52) for the N-particle time-dependent density matrix in terms of a product of three (anti-) symmetrised time-evolution amplitudes, normalised by the N-particle partition function, led to the expression (4.62) for the density matrix of N particles in terms of a product of one-particle ones.

In the following Section 4.6, we calculated the N-particle partition function from the trace (4.64) of the N-particle time-evolution amplitude. In contrast to the two-particle case, we now had to integrate a sum of $N!$ products of permutation dependent one-particle time-evolution amplitudes, which had the explicit form of the N-dimensional Gaussian integral (4.66) with permutation-dependent matrices of the form (4.73). In order to solve this integral, we had to find an expression for the corresponding permutation-dependent determinants. As these matrices consist of a linear combination of the corresponding permutation matrix and its inverse, they obey the same similarity relation as the permutation matrices themselves. Secondly, we observed that for every similarity class of permutation matrices, there is at least one matrix of the form (4.73) that is block diagonal. Since all permutation matrices within the same similarity class share the same determinant, and as the determinant of a block diagonal matrix factorises into the determinants of the constituent sub-matrices, there is a cycle decomposition of the above permutation-dependent determinants into per n-cycle determinants of single-cycle matrices (4.73). Thus, in the next step, we had to find the general expression for the determinant of a single-n-cycle matrix. To this end, we performed a Laplace expansion of the special single-cycle determinant (4.79), which yielded the difference equation (4.86) in terms of only the determinant of a tridiagonal matrix. As a consequence, we only had to find the general solution of its difference equation (4.81), which we obtained in closed form by performing a Z-transform, the properties of which are summarised in Appendix A. Using the general solution (4.106) then yielded the N-particle canonical partition function in cycle-reduced form (3.100).

In Section 4.7 we calculated the reduced time-dependent one-particle density matrix in an N-particle ensemble as a recursion analogous to that for the canonical partition function. Here, however, contributions from broken cycles (4.109) appeared and we first had to derive the master equation (4.114) in order to further evaluate the reduced density matrix, for which we then obtained the recursion (4.115). From this, it was straightforward to calculate the corresponding reduced time-dependent one-particle width in an N-particle using only the one-particle results. For said width, we obtained the recursion (4.117), which, as in the one-particle case, factorised into a product of the thermodynamic one-particle width and the above time-dependent function (4.19).

We displayed a plot of the time-independent part in Fig. 4.4 for bosons, as well as for fermions. For bosons, the curves for N particles have the same general behaviour as the one-particle width: they start off at one half the oscillator width squared and approach linear asymptotes of equal slope in the high-temperature limit. However for particle numbers N greater than one, these asymptotes have lower lying and N-dependent y-intercepts. For fermions the picture is similar, with the exception that now the asymptotes have positive N-dependent intercepts, and consequently the reduced width starts off at N times the value for bosons. In the following, we derived the form of these intercepts for bosons and fermions by starting with the ansatz (4.121) for the N-particle partition function and deriving the recursion relation (4.124) for the unknown coefficients. We obtained its solution (4.142) via the generating function method and inserting this into the reduced one-particle width (4.117) finally yielded the expression (4.142) for the above asymptotes.

Chapter 6

Outlook

The work that was presented in this thesis has only laid the foundations for the treatment of the simple non-equilibrium phenomenon of a trap-frequency quench in the canonical formalism. Thus, it is by no means complete and there remain many interesting questions to be pursued. In this outlook we will give a brief overview of some ideas for the generalisation end extension of the present work.

We start with the most obvious generalisation, namely the inclusion of weak particle interactions, which would enable the comparison of results between theory and present as well as future experiments. This may be done by generalising the canonical perturbation theory that is presented in Ref. [31] to density matrices. In the following, we briefly outline this ansatz. In the many-particle path-integral formalism, the imaginary-time evolution amplitude for a weakly interacting Bose system is given by the following N-fold path-integral:

$$(x_1, \ldots, x_N \mid x_1', \ldots, x_N')_{\text{int}}^{(+)} = \frac{1}{N!} \sum_P \prod_{n=1}^{N} \left[\int_{x_n(\tau_a)=x_n'}^{x_n(\tau_b)=x_{P(n)}} \mathcal{D}x_n(\tau) \right] \times \exp\left\{ -\frac{1}{\hbar} \Big(\mathcal{A}^{(0)}[x_1, \ldots, x_N] + \mathcal{A}^{(\text{int})}[x_1, \ldots, x_N] \Big) \right\} , \tag{6.1}$$

where

$$\mathcal{A}^{(0)}[x_1, \ldots, x_N] = \sum_{n=1}^{N} \int_{\tau_a}^{\tau_b} d\tau \left[\frac{M}{2} \dot{x}_n^2(\tau) + V(x_n(\tau)) \right] \tag{6.2}$$

is the free part of the Euclidean action, and

$$\mathcal{A}^{(\text{int})}[x_1, \ldots, x_N] = \frac{1}{2} \sum_{n,m=1}^{N} \int_{\tau_a}^{\tau_b} d\tau \, V^{(\text{int})}\Big(x_n(\tau) - x_m(\tau) \Big) \tag{6.3}$$

is the interaction part. Here we note that any self-interaction is to be avoided, i.e. $n \neq m$ and that the interaction is modelled by a contact s-wave scattering potential of the form $V^{(\text{int})}(x) = (4\pi\hbar^2 a_{\text{s}}/M)\delta(x)$, with the s-wave scattering length a_{s}. We then obtain the perturbation expansion of the interacting bosonic N-particle amplitude (6.1) simply by Taylor expanding the exponential that contains the interaction part (6.3). Of course, the fundamental quantities that interact in (6.1) are the permutation cycles. For example, in the above amplitude for the case of the partition function, and in first order, we have one contribution per n-cycle that comes from the single interaction between two different cycles, and one contribution per n-cycle that comes from the interaction of the cycle with itself. Here it remains to be worked out, how this approach can be used to describe a trap-frequency quench.

Another interesting aspect would be to have two quenched BECs close together and to study the interactions between both. Modelling this situation could be interesting for the study of large atomic nuclei.

Also, recalling the discussion in the introduction to non-equilibrium phenomena in Section 1.2, we must remind ourselves that a quench cannot allways be considered as taking place instantly. Consequently, we must assume that the quench happens on a short but finite timescale δt_{q}. It would then be interesting to investigate the effect of said timescale on the resulting dynamics after the quench has taken place.

Last, in our approach we have assumed that the equilibrium density matrix evolves in time according to the usual unitary, i.e. reversible quantum dynamics given by the Von-Neumann equation (4.3). Another interesting field would be opened by dropping the assumption of unitary dynamics in favour of the very general non-unitary and thus irreversible dynamics of the Lindblad type. The Lindblad equation or master equation in the Lindblad form,

$$\frac{d}{dt}\hat{\varrho}(t) = -\frac{i}{\hbar}\big[\hat{H}, \hat{\varrho}(t)\big] + \frac{1}{2\hbar}\sum_{i}\Big(\big[\,\hat{V}_j\hat{\varrho}(t), \hat{V}_j^{\dagger}\,\big] + \big[\,\hat{V}_j, \hat{\varrho}(t)\hat{V}_j^{\dagger}\,\big]\Big) \ , \tag{6.4}$$

is the most general type of Markovian and time-homogeneous master equation describing the non-unitary, i.e. dissipative evolution of the density operator that is trace preserving and completely positive. In (6.4), the operators $\hat{V}_j$ represent the coupling of the dissipative environment to the density operator $\hat{\varrho}(t)$. There are no further general restrictions on these operators and their choice in physical applications is often heuristic.

Appendix A

Z-Transform

In nature and technology, one can distinguish between discrete and continuous processes. Whereas many continuous processes may be described mathematically by differential equations, the description of discrete ones often leads to difference equations or recursion relations. Differential equations are most easily solved by taking the Fourier or Laplace transforms for periodic and non-periodic processes respectively, whereas for difference equations, more suitable operator methods were developed; the most well known of which is the Z-transform, which is closely related to the Laplace transform.

The Z-transform [32] was introduced, under this name, by Ragazzini and Zadeh in 1952 [33]. The so-called modified or advanced Z-transform, that we refer to in the following, was later developed by E. I. Jury, and is presented in his book [34]. He writes:

> The techniques of z-transform method are not new, for they can actually be traced back as early as 1730 when DeMoivre [35] introduced the concept of the "generating function" (which is actually identical to the z-transform) to probability theory.

In the following, we briefly summarise the main properties of the Z-transform which will be useful for solving the recursion relation (4.81) for the determinant T_n of the tridiagonal matrix.

A.1 Formal Power Series and the Generating Function Method

The notion of formal power series allows one to employ much of the analytical machinery of power series in settings that do not have natural notions of convergence. A generating function is then a formal power series whose coefficients encode information about a sequence that is indexed by the natural numbers. The idea behind the generating function method is thus both simple and powerful: Given some equation involving sequences, e.g. recursion relations or difference equations etc., such as

$$a_n = b_n + c_n + d \ , \qquad \text{where } n \in \mathbb{N}, \tag{A.1}$$

we may turn it into an equation of holomorphic functions by multiplying the whole equation by a complex variable z, and formally summing (A.1) from zero, or some other starting number, such as 1, to infinity:

$$\sum_{n=0}^{\infty} a_n z^n = \sum_{n=0}^{\infty} b_n z^n + \sum_{n=0}^{\infty} c_n z^n + d \sum_{n=0}^{\infty} z^n \ . \tag{A.2}$$

Thus, the power series in (A.2) uniquely defines holomorphic functions on the complex plane, so by this straightforward manipulation we have effectively "transformed" our original equation

(A.1) from the discrete n-domain into the continuous complex z-domain:

$$A(z) = B(z) + C(z) + D(z) \;, \qquad \text{where} \quad A(z) = \sum_{n=0}^{\infty} a_n z^n \;, \text{ etc.} \tag{A.3}$$

This allows us to use the whole machinery of complex analysis to solve our problem.

A.2 *Z*-Transform: Definition and Properties

The Z-transform converts a discrete n-domain signal, which is a sequence of real or complex numbers, into a complex frequency-domain representation. The series

$$Y(z) = \sum_{n=0}^{\infty} y_n \, z^{-n} \tag{A.4}$$

is assigned to the sequence $\{y_n\}$. If the above series is convergent, the sequence y_n is said to be Z-transformable and, thus, the Laurent series $Y(z) = \mathcal{Z}\{y_n\}$ defines a holomorphic function on the field of complex numbers, which is called the Z-transform of $\{y_n\}$. For every Z-transformable sequence $\{y_n\}$, there exists a number $R \in \mathbb{R}$, such that for $|z| > R^{-1}$ the Laurent series (A.4) converges absolutely and diverges for $|z| < R^{-1}$. Here, R is called the region of convergence (ROC) of (A.4) with respect to z^{-1}. If the above Laurent series converges for all $|z| > R^{-1}$, we define $R = \infty$. In contrast, if the sequence is not Z-transformable, we set $R = 0$.

The Z-transform has the following properties, which follow straightforwardly from its definition (A.4):

1. Linearity For all constants a and b it holds that

$$\mathcal{Z}\{a\, y_n + b\, x_n\} = a\, Y(y_n) + b\, Y(x_n) \;. \tag{A.5}$$

2. First Translation Theorem

$$\mathcal{Z}\{y_{n-k}\} = \; z^{-k}\, Y(z) \qquad k = 0, 1, 2, \dots \;, \tag{A.6}$$

where we have made the obvious definition $y_{n-k} = 0$ for $n - k < 0$.

3. Second Translation Theorem

$$\mathcal{Z}\{y_{n+k}\} = \; z^k \left[Y(z) - \sum_{\nu=0}^{k-1} y_\nu \, z^{-\nu} \right] \qquad k = 1, 2, \dots \tag{A.7}$$

Here, the coefficients y_ν in the sum on the right side are the initial values of the difference equation.

4. Scaling in the *Z*-domain

$$\mathcal{Z}\{a^n \, y_n\} = Y\left(a^{-1}\, y_n\right) \tag{A.8}$$

5. Summation For $|z| > \max\{1, R^{-1}\}$ we have

$$\mathcal{Z}\left\{\sum_{\nu=0}^{n-1} y_\nu\right\} = \frac{1}{z-1} Y(y) . \tag{A.9}$$

6. Differentiation

$$\mathcal{Z}\{n\, y_n\} = -z \frac{d}{dz} Y(z) . \tag{A.10}$$

7. Integration Under the condition that $y_0 = 0$, we have

$$\mathcal{Z}\left\{n^{-1}\, y_n\right\} = \int_z^\infty \frac{Y(\zeta)}{\zeta}\, d\zeta . \tag{A.11}$$

8. Convolution The discrete convolution of two sequences $\{x_n\}$ and $\{y_n\}$ is defined as the operation

$$x_n * y_n = \sum_{\nu=0}^{n} x_\nu\, y_{n-\nu} . \tag{A.12}$$

In case the Z-transforms $\mathcal{Z}\{x_n\} = X(z)$ with ROC R_x, and $\mathcal{Z}\{y_n\} = Y(z)$ with ROC R_y exist, it holds that

$$\mathcal{Z}\{x_n * y_n\} = X(z) Y(z) , \tag{A.13}$$

for $|z| > \max\{R_x^{-1}, R_y^{-1}\}$. This corresponds to the Cauchy product of two series.

A.3 Inverse *Z*-Transform

The application of the inverse Z-transform corresponds to finding the unique original sequence $\{y_n\}$ of the holomorphic z-domain function $Y(z)$ from (A.4), which we write as $\mathcal{Z}^{-1}\{Y(z)\} = \{y_n\}$. For transforming back to the n-domain there are several methods:

1. Via the Laurent series of $Y(z)$, provided that the Laurent series is known or can be easily determined. The contour integral

$$y_n = \mathcal{Z}^{-1}\{Y(z)\} = \frac{1}{2\pi i} \oint_C Y(z)\, z^{n-1} dz \tag{A.14}$$

   yields y_n as the residues of $Y(z) z^{n-1}$, where the contour C is to be taken counterclockwise, encircling the origin and all of the poles of $Y(z)$, and lying entirely in the region of convergence.

2. Via the Taylor series of $Y(1/z)$. As $Y(1/z)$ is a power series in raising powers of z, and because of the definition (A.4) of $Y(z)$, we obtain y_n from the Taylor formula

$$y_n = \frac{1}{n!} \frac{d^n}{dz^n} Y\left(\frac{1}{z}\right)\bigg|_{z=0} \qquad \text{for} \quad n = 1, 2, \ldots \tag{A.15}$$

3. By using limit theorems. In analogy to the limit theorems for the Laplace transform of a function, the following limit theorems hold for the Z-transform $Y(z) = \mathcal{Z}\{y_n\}$ of a sequence $\{y_n\}$:

$$y_0 = \lim_{z\to\infty} Y(z) \ , \qquad y_1 = \lim_{z\to\infty} \mathcal{Z}\{Y(z) - y_0\} \ , \qquad y_2 = \lim_{z\to\infty} \mathcal{Z}\{Y(z) - y_0 - y_1 z^{-1}\}, \dots \tag{A.16}$$

   Thus, we obtain the original sequence $\{y_n\}$ from $Y(n)$. The above statement is also known as *initial value theorem.* If and only if the limit $\lim_{z\to\infty} y_n$ exists, the corresponding final value theorem reads

$$\lim_{n\to\infty} y_n = \lim_{n\to 1+0} (z-1)Y(z) \ . \tag{A.17}$$

4. By using tables of Z-transform pairs. Many common pairs of sequences and their respective Z-transforms are tabulated(see e.g. [32]). Here, one tries to write $Y(z)$ as a sum,

$$Y(z) = Y_1(z) + Y_2(z) + Y_3(z) + Y_4(z) + \dots \ , \tag{A.18}$$

   where for all terms $Y_i(z)$ the inverse Z-transform y_i is known. With the linearity property (A.5) one then obtains

$$y_n = y_n^{(1)} + y_n^{(2)} + y_n^{(3)} + y_n^{(4)} + \dots \ . \tag{A.19}$$

5. By writing $Y(z)$ in terms of partial fractions and the transforming back to the n-domain. This method is important, as it often allows one to obtain a solution in closed form of difference equations and recursions.

A.4 Relation to Fourier and Laplace Transforms

The so-called *bilateral* Z-transform is the two-sided, doubly infinite Z-transform defined by

$$Y^{(2)}(z) = \mathcal{Z}^{(2)}\left\{\{y_n\}_{n=-\infty}^{\infty}\right\} = \sum_{n=-\infty}^{\infty} y_n\, z^{-n} \ . \tag{A.20}$$

The bilateral transform is generally less commonly used than the unilateral Z-transform, since only the latter finds widespread application as a technique essentially equivalent to generating functions, as was discussed above. By evaluating the bilateral Z-transform at $z = \mathrm{e}^{i\omega}$, i.e. on the unit circle, we obtain the discrete version of the Fourier transform, which is referred to as the *discrete-time Fourier transform* (DTFT). Thus, the bilateral Z-transform is a generalisation of the DTFT.

If we describe a discrete function $y(t)$ as step function, we have

$$y(t) = y(nT) = y_n \ , \qquad \text{for} \quad nT \le t < (n+1)T \qquad n = 1, 2, \dots \ , \tag{A.21}$$

so $y(t)$ is continuous and constant inbetween the *sampling points* nT. We may then apply the Laplace transform $\mathcal{L}$ to this piecewise continuous function, which yields for $T = 1$:

$$\mathcal{L}\left\{y(n)\right\} = Y(p) = \sum_{n=0}^{\infty} \int_{n}^{n+1} dt\, y_n\, \mathrm{e}^{-nt} = \sum_{n=0}^{\infty} y_n \, \frac{\mathrm{e}^{-np} - \mathrm{e}^{-(n+1)p}}{p} = \frac{1 - \mathrm{e}^{-p}}{p} \sum_{n=0}^{\infty} y_n\, \mathrm{e}^{-np} \ . \tag{A.22}$$

The infinite series in (A.22) is known as the discrete Laplace transform of a sequence y_n and is denoted by the symbol $\mathcal{D}$:

$$\mathcal{D}\left\{y(n)\right\} = \mathcal{D}\left\{y_n\right\} = \sum_{n=0}^{\infty} y_n \, \mathrm{e}^{-np} \; . \tag{A.23}$$

If in (A.23) one sets $z = \mathrm{e}^p$, the Z-transform (A.4) is recovered. This leads to the following relationship between the Laplace and Z-transforms for step functions:

$$p\,Y(p) = \left(1 - \frac{1}{z}\right) Y(z) \; , \qquad \text{i.e.} \qquad p\,\mathcal{L}\left\{y(t)\right\} = \left(1 - \frac{1}{z}\right) \mathcal{Z}\left\{y_n\right\} \; . \tag{A.24}$$

Bibliography

[1] S. N. Bose, *Plancks Gesetz und Lichtquantenhypothese*, Zeitschrift für Physik **26**, 178 (1924)

[2] A. Einstein, *Quantentheorie des einatomigen idealen Gases*, Sitzber. Kgl. Preuss. Akad. Wiss., 261 (1924)

[3] A. Einstein, *Quantentheorie des einatomigen idealen Gases*, *Zweite Abhandlung*, Sitzber. Kgl. Preuss. Akad. Wiss., 3–14 (1925)

[4] M. H. Anderson, J. R. Ensher, M. R. Matthews, C. E. Wieman, and E. A. Cornell, *Observation of Bose-Einstein Condensation in a Dilute Atomic Vapor*, Science, **269**, 198 (1995)

[5] W. Ketterle, D. S. Durfee, and D. M. Stamper-Kurn, *Making, probing and understanding Bose-Einstein condensates*, Proceedings of the International School of Physics "Enrico Fermi", Course CXL, edited by M. Inguscio, S. Stringari and C.E. Wieman, (IOS Press, Amsterdam, 1999) p. 67.,
arxiv:cond-mat/9904034

[6] C. C. Bradley, C. A. Sackett, J. J. Tollett, and R. G. Hulet, *Evidence of Bose-Einstein Condensation in an Atomic Gas with Attractive Interactions*, Phys. Rev. Lett. **75**, 1687 (1995)

[7] K. B. Davis, M.-O. Mewes, M. R. Andrews, N. J. van Druten, D. S. Durfee, D. M. Kurn, and W. Ketterle, *Bose-Einstein Condensation in a Gas of Sodium Atoms*, Phys. Rev. Lett. **75**, 3969 (1995)

[8] M. Greiner, O. Mandel, T. Esslinger, T. W. Hänsch and I. Bloch, *Quantum Phase Transition from a Superfluid to a Mott Insulator in a Gas of Ultracold Atoms*, Nature **415**, 39 (2002)

[9] I. Bloch, *Ultracold Quantum Gases in Optical Lattices*, Nature Physics **1**, 23 (2005)

[10] D. Jaksch, C. Bruder, J. I. Cirac, C. W. Gardiner and P. Zoller, *Cold Bosonic Atoms in Optical Lattices*, Phys. Rev. Lett. **81**, 3108 (1998)

[11] M. Greiner, O. Mandel, T. Hänsch and I. Bloch, *Collapse and revival of the matter wave field of a Bose-Einstein condensate*, Nature **419**, 51 (2002)

[12] C. Kollath, A.M. Läuchli and E. Altman, *Quench Dynamics and Nonequilibrium Phase Diagram of the Bose-Hubbard Model*, Phys. Rev. Lett. **98**, 180601 (2007)

[13] E. Santos and A. Pelster, in preparation

[14] B. Bradlyn, F. E. A. dos Santos, and A. Pelster, *Effective Action Approach for Quantum Phase Transitions in Bosonic Lattices*, Phys. Rev. A **79**, 013615 (2009)

[15] L. Pitaevskii and S. Stringari, *Bose-Enstein Condensation*, Oxford Science Publications, Clarendon Press, Oxford, 2003

[16] C. J. Pethick and H. Smith, *Bose-Einstein Condensation in Dilute Gases*, 2nd. Ed., Cambridge University Press, Cambridge, 2008

[17] A. Griffin, T. Nikuni and E. Zaremba, *Bose-Condensed Gases at Finite Temperatures*, Cambridge University Press, Cambridge, 2009

[18] M. Hamermesh, *Group Theory and its Application to Physical Problems*, Addison-Wesley, London, 1962

[19] J. S. Lomont, *Applications of Finite Groups*, 3rd. Ed., Academic Press, New York, London, 1970

[20] W.-K. Tung, *Group Theory in Physics*, World Scientific, Singapore, 1985

[21] V. Krishnamurthy, *Combinatorics–Theory and Applications* Wiley, New York, 1986

[22] H. Kleinert, *Path Integrals in Quantum Mechanics, Statistics, Polymer Physics and Financial Markets*, 5th Ed., World Scientific, Singapore, 2008

[23] W. Pauli, *The Connection Between Spin and Statistics*, Phys. Rev. **58**, 716 (1940)

[24] W. Nolting, *Fundamentals of Many-Body Physics Principles and Methods*, Springer-Verlag, Berlin, Heidelberg, 2009

[25] C. DeWitt-Morette, *On the Definition and Approximation of Feynman's Path Integrals*, Phys. Rev. **81**, 848 (1951)

[26] A. Pelster, *Bose-Einstein-Kondensation*, lecture notes (in German), Universität Duisburg-Essen, 2004

[27] K. Glaum, H. Kleinert, and A. Pelster, *Condensation of ideal Bose gas confined in a box within a canonical ensemble*, Phys. Rev. A **76**, 063604 (2007)

[28] F. Brosens, J. T. Devreese and L. F. Lemmens, *Thermodynamics of coupled identical oscillators within the path-integral formalism* Phys. Rev. E **55**, 227 (1997)

[29] W. Korolevski, *Bose-Einstein-Kondensation in kanonischen Ensembles* (in German) Diploma thesis, Freie Universität Berlin, 2009

[30] K. Glaum, *Bose-Einstein-Kondensation in endlichen Systemen* (in German) PhD thesis, Freie Universität Berlin, 2008
`http://www.diss.fu-berlin.de/2008/117/index.html`

[31] K. Glaum, A. Pelster and H. Kleinert, *Thermodynamical Properties for Weakly Interacting Dipolar Gases Within Canonical Ensemble* in W. Janke and A. Pelster (Editors): Proceedings of the 9th International Conference Path Integrals – New Trends and Perspectives; Max-Planck Institute for the Physics of Complex Systems, Dresden, Germany, September 23–28, 2007; World Scientific, 403-408 (2008)

[32] I. A. Bronstein, K. A Semendjajew, G. Musiol and H. Mühlig, *Taschenbuch der Mathematik* (in German) 3rd Ed., Verlag Harry Deutsch, Frankfurt am Main, 1997

[33] L. A. Zadeh and J.R. Ragazzini, *The Analysis of Sampled-Data Systems*, Applications and Industry (AIEE) **1**, 224-234, (1952)

[34] E. I. Jury, *Theory and Application of the z-Transform Method*, John Wiley & Sons, 1964

[35] A. de Moivre, *Miscellanes Analytica de Seriebus et Quatratoris* (in Latin), London, 1730

Acknowledgements

First of all, I am much obliged to Priv.-Doz. Dr. Axel Pelster for supervising my thesis. He always took the time to help me out when I was lost in the hell of never ending, erroneous calculations. His ability to find mistakes, being able to adapt to every handwriting and mathematical notation in seconds, is legendary and his enthousiasm and motivation, paired with mathematical knowledge and experience as a supervisor helped me enormously during the last year. Additionally, I am grateful that he spent his weekends and his vacation with correcting the manuscript of this thesis.

I would also like to thank Prof. Dr. Dr. h.c. mult. Hagen Kleinert for giving me the opportunity to work on my thesis in his group. His physical insight and his ability to intuitively explain advanced topics from quantum field theory, general relativity and cosmology in simple terms has helped me greatly in “getting the big picture”, i.e. in understanding the foundations of modern theoretical physics. Of course, I also want to thank Annemarie Kleinert, who, together with her husband and Michael, hosted the group’s garden party in August.

I would like to thank my former room mates Matthias Ohliger and Tobias Graß, as well as my later room mates Walja Korolevski, Nathalie Pfitzinger and Hendrik Ludwig for their help and for all the useful discussions concerning theoretical physics and the universe in general. Here, special thanks go to Walja for spending her afternoon diving into my calculations and finding the bug in my programme. Furthermore, I very much enjoyed the pleasant working atmosphere during my time in the AG-Kleinert. This might have been due in part to the strong Brasilian ”vibrations”. Thus, I am grateful to my Brasilian colleagues Victor Bezerra, Aristeu Lima, Francisco Ednilson Alves dos Santos and Flavio Nogueira for causing these vibrations. Additional thanks go to Jürgen Dietel for answering my numerous questions concerning the permutation group and for our long discussions about his own work, about stocks, investment and many other things. I also want to thank Ednilson and Victor for reading part of the manuscript and, last but not least, my very special thanks go to Graeme Cunningham for proofreading it and correcting the spelling and english grammar mistakes.