Rheinland-Pfälzische Technische Universität Kaiserslautern Landau

Master Thesis

Bogoliubov Theory of Bose Gases in Finite Quasi 2D Systems

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Abstract

A class of bosonic quantum gases is subjected to a detailed theoretical treatment. Second quantized Schrödinger field theory and an extension of the grand canonical ensemble serve as the fundamental quantum mechanical and statistical models. On that basis, the fundamental equations for classical thermodynamics are derived using a generalized Bogoliubov theory. Exemplary thermodynamical calculations are performed for the Bose gas in a two-dimensional box and on the surface of a sphere. The three focal points of the thesis are trapping geometry (confining the particles to lower-dimensional manifolds), weak (isotropic pairwise) interaction and superfluidity. Extensive supplementary material on ensemble theory, differential geometry and regularization is provided to improve intuition for and to mathematically support the applied techniques and models.

Eine Klasse von bosonischen Quantengasen wird einer detaillierten theoretischen Behandlung unterzogen. Zweitquantisierte Schrödinger Feldtheorie und eine Erweiterung des großkanonischen Ensembles dienen als die fundamentalen quantenmechanischen und statistischen Modelle. Auf ihrer Basis werden die fundamentalen Gleichungen der klassichen Thermodynamik mittels einer generalisierten Bogoliubov Theorie hergeleitet. Beispielhafte thermodynamische Berechnungen werden am Bosegas in der zweidimensionalen Box und auf der Oberfläche einer Kugel durchgeführt. Die drei Schwerpunkte der Arbeit sind die Fallengeometrie (das Einsperren von Teilchen auf niederdimensionalen Mannigfaltigkeiten), schwache (isotrope paarweise) Wechselwirkung und Suprafluidität. Umfangreiches Zusatzmaterial zu Ensembletheorie, Differentialgeometrie und Regularisierung wird zur Verfügung gestellt, um die Intuition für die angewandten Techniken und Modelle zu verbessern und diese mathematisch zu unterfüttern.

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Lastly, I want to thank Prof. Dr. Michael Fleischhauer for agreeing to be the second assessor and for hosting a presentation of my results in his working group.

Statement of authorship

I hereby affirm that I have independently written the enclosed master's thesis with the title "Bogoliubov Theory of Bose Gases in Finite Quasi 2D Systems" and have not used any sources and aids other than those indicated, and that I marked quotations accordingly.

Kaiserslautern, December 2023

Til Möhnen

Contents

1 Introduction

This introductional section embeds the present thesis into the broader context of the field of research on cold quantum gases. First a rough account of the historical development of the field is given, highlighting its explosive growth in the last decades. Afterwards the experimental concern of trapping neutral atoms is covered, focusing on the creation of box- and shell-shaped gases. Lastly, the structure of the thesis is layed out.

1.1 Historical developments

The first experiment showcasing a purely quantum statistical phenomenon was conducted by Pjotr Kapiza [1] in 1938, where a vanishingly small viscosity was measured in liquid helium below the lambda point (at approximately 2.17K), indicating a new phase of matter later labeled a superfluid. The Bose-Einstein condensate, which constitutes another phase of matter, had already been predicted in 1924 by Albert Einstein [2] on the basis of Satyendranath Boses [3] quantum statistical considerations. In comparison to the superfluid however, an experimental realization of Bose-Einstein condensation only succeeded six decades later in 1995, when Wieman et al. [4] cooled a gas of rubidium-87 below 170nK using laser cooling and evaporative cooling and were able to identify the characteristic spike at the origin in the momentum distribution of their sample.

At this crucial point in time, experimental techniques had finally been developed to a degree that paved the way for the investigation of the rich physics of ultracold quantum gases. The field has greatly expanded ever since – particularly on the experimental front – with experiments exploring various aspects from equilibrium properties (like Bose-Einstein condensation) over perturbative phenomena (like sound propagation) to non-equilibrium properties (like critical phenomena). Experiments with both fermions and bosons [5, 6, 7] have been performed in one-, two- and three-dimensional box traps; and gases with long-range short-range and unisotropic pairwise interactions have been realized; just to name a few achievements. This industriousness on the experimental front has yet to be fully matched by its theoretical counterpart, an endeavour to which this thesis aims at contributing.

1.2 Trapping neutral atoms

The experimental aspect of generating trapping potentials for neutral atoms shall be briefly illuminated, as trapping geometry will play a key role in the present thesis. Many different trapping potentials have been realized for cold quantum gases, e.g. harmonical traps and optical lattices. Here, only the generation of box- and shell-shaped potentials is discussed.

1.2.1 Gravity

Gravity has proven to be an obstacle universally present in ultracold atomic gases. The average thermal energy of the confined atoms usually lies orders of magnitude below the increase of their gravitational potential across the trap, which leads to a pooling of the atoms at the bottom of the trap. Several techniques have been applied to mitigate this gravitational sag. Attempts are being made to negate gravity by superposing a linear optical potential [8], which still proves to be a challenging task on typical experimental length scales. Another solution lies in subjecting the entire experimental setup to free fall in facilities like the Bremen drop tower [9]. The most recent and arguably most impressive approach lies in relocating the experiment to an orbit around earth, such that perpetual freefall is achieved; which was realized in 2018 with the installation of the cold atom lab (CAL) aboard the ISS [10].

1.2.2 Box traps

Optical box traps confine atoms to a polyhedral volume (typically a cuboid) by providing a potential that vanishes in its interior and has steep and high walls on the boundary. The potential generation is based on light-matter intraction as it is used in optical dipole traps: A time average of the interaction of an electric field with the oscillating dipoles induced in an atom by that same field produces an effective potential, which is essentially proportional to the intensity of the light. The mechanism is briefly explained in the following.

Here, the effect of an external electric field on an electron inside an atom is described qualitatively by a classical toy model. A homogenous external field

$$E(t) = E_0 \cos(\omega t), \tag{1.1}$$

with amplitude $E_0 \in \mathbb{R}$ and frequency $\omega \in [0, \infty]$ is assumed, that influences the electron via the Lorentz force. Furthermore, the electron is assumed to experience an approximately harmonic potential (characterized by a frequency ω_0) due to its' interaction with the atomic body. The electron's trajectory $x(t)$ is then described by a driven harmonic oscillator

$$\frac{e}{m}E = \frac{d^2}{dt^2}x + \omega_0^2 x, \tag{1.2}$$

with e and m denoting the electron's charge and mass, respectively. The differential equation (1.2) is solved by

$$x(t) = \frac{e}{m}E_0 \frac{1}{\omega_0^2 - \omega^2} \cos(\omega t). \tag{1.3}$$

The atom's induced dipole moment $ex(t)$ has the potential energy $ex(t) \cdot E(t)$ in the external field and a time average over the period $\frac{2\pi}{\omega}$ yields the energy

$$U = \frac{e^2 \|E_0\|^2}{2m} \frac{1}{\omega_0^2 - \omega^2}. \tag{1.4}$$

This energy is essentially proportional to the intensity of the ligh and is positive/negative for blue-/red-detuned ($\omega > \omega_0 / \omega < \omega_0$) light. In reality the electric field is obviously not homogenous, however it varies on lengthscales far greater than the expanse of the electron's wave function. A slow atom therefore adiabatically follows the spatially dependent potential U.

Optical boxes are typically constructed with "flat" laser beams, which have a line as their cross section, so-called sheet beams. A set of blue detuned sheet beams is used to create the repulsive walls of the box trap. The generation of box traps was greatly facilitated by the implementation of spatial light modulators, in particular the digital mirror device (DMD), in experimental setups. DMDs are programmable two-dimensional arrays of $\sim 10^6$ tiltable mirrors, which are used to imprint arbitrary intensity patterns into the cross section of a laser beam.

1.2.3 Bubble traps

Bubble traps confine atoms to a thin shell by providing a trapping potential that takes its minimum on some closed surface. Typical magnetic traps rely on the interaction of the magnetic moment of the contained atoms with a static external magnetic field B, providing a potential that is essentially proportional to the norm $\|B\|$. Assuming that this potential is minimal on some closed surface ∂V, it must attain a maximum at some point inside the volume V enclosed by that surface. This is impossible in the absence of charge currents inside V and for a static magnetic field, as is shown in the following.

As a necessary condition for $\|B\|$ to attain a maximum, its Hessian matrix H must become negative definite. Consequently, all eigenvalues of H have to be negative. This implies that the trace of H has to be negative, i.e.

$$0 < \mathrm{Tr}(H), \tag{1.5}$$

which is now led to a contraction. Inside the trap, the magnetic field obeys the Maxwell equations

$$\nabla \cdot B = 0 \quad \wedge \quad \nabla \times B = 0. \tag{1.6}$$

In conjunction they imply the auxiliary result

$$0 = \nabla \times (\nabla \times B) = \nabla (\nabla \cdot B) - \Delta B = -\Delta B. \tag{1.7}$$

Therewith, the trace of H evaluates to

$$\mathrm{Tr}(H) = \Delta\|B\| = \frac{1}{2\|B\|}\nabla\cdot\nabla\sum_{i=1}^{3}B_i^2 = \frac{1}{\|B\|}\sum_{i=1}^{3}\Big(\|\nabla B_i\|^2 + B_i\Delta B_i\Big) = \frac{1}{\|B\|}\sum_{i=1}^{3}\|\nabla B_i\|^2 \geq 0, \quad (1.8)$$

which contradicts the maximum condition (1.5). It is consequently impossible to realize a bubble trap using only static magnetic fields. A workaround to this problem was already suggested in 2001 by Zobay and Garraway [11], who proposed to confine atoms via field-induced adiabatic potentials. Due to the aforementioned gravitational sag, experimental realizations have only been possible in recent years. In the following, an introduction to field-induced adiabatic potentials is provided (essentially based on [12]).

The basic concept is to introduce a dynamic magnetic field B_1 in addition to the static field B_0, such that time averaging approximately yields an effective potential, that can attain a maximum. The magnetic moment in the external magnetic field is modeled by the semiclassical Rabi model, which describes the atom in a first quantized way while the light is modeled as a classical external magnetic field.

The spatial dependency is ignored at first. Thus, without loss of generality, the static field B_0 is chosen to be oriented in the (local) z-direction like

$$B_0 = b_0 e_z, \quad (1.9)$$

with amplitude $b_0 \in [0, \infty[$ and the dynamic field B_1 is expressed in spherical coordinates like

$$B_1(t) = b_1 \begin{pmatrix} \cos(\varphi)\sin(\vartheta) \\ \sin(\varphi)\sin(\vartheta) \\ \cos(\vartheta) \end{pmatrix} \cos(\omega t), \quad (1.10)$$

with amplitude $b_1 \in [0, \infty]$, radio frequency ω and angles $\varphi \in [0, 2\pi[$ and $\vartheta \in [0, \pi]$. Further, the magnetic moment of the atom is given in terms of the total angular momentum operator $\hat{F}$, which has the usual defining commutation relations

$$\left[\hat{F}_i, \hat{F}_j\right] = i\hbar\sum_k \varepsilon_{ijk}\hat{F}_k, \quad (1.11)$$

with $i, j, k \in \{1, 2, 3\}$ (or equivalently $i, j, k \in \{x, y, z\}$). Its interaction with the magnetic field is then modeled by a Hamilton operator of the form

$$\hat{H} = \frac{g_F\mu_\mathrm{B}}{\hbar}\hat{F}\cdot(B_0 + B_1(t)) \quad (1.12)$$

and the time evolution of the atom's state $|\psi(\bullet)\rangle$ is given by the Schrödinger equation

$$i\hbar\frac{d}{dt}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle. \quad (1.13)$$

By applying a unitary transformation $\hat{R}$ with $\hat{R}^\dagger\hat{R} = 1$ to the atom's state like

$$|\psi(t)\rangle_\mathrm{rot} \equiv \hat{R}^\dagger|\psi(t)\rangle, \quad (1.14)$$

an equivalent differential equation

$$i\hbar\frac{d}{dt}|\psi(t)\rangle_\mathrm{rot} = \hat{H}_\mathrm{rot}|\psi(t)\rangle_\mathrm{rot} \quad (1.15)$$

is found, with a transformed Hamilton operator

$$\hat{H}_\mathrm{rot} \equiv -i\hbar\hat{R}^\dagger\left(\frac{d}{dt}\hat{R}\right) + \hat{R}^\dagger\hat{H}\hat{R}. \quad (1.16)$$

The specific operator $\hat{R}$ useful in the given setup is a time dependent rotation and reads

$$\hat{R} \equiv e^{\frac{s\omega t}{i\hbar}\hat{F}_z}, \quad (1.17)$$

where $s \equiv \mathrm{sgn}(g)$ denotes the signum of the Landé g-factor. In preparation of the evaluation (1.16) at (1.17), an auxiliary calculation is necessary. The operators

$$\hat{F}_\pm = \hat{F}_x \pm i\hat{F}_y, \tag{1.18}$$

are defined, which exhibit the commutation relation

$$\left[\hat{F}_\pm, \hat{F}_z\right] = \mp\hbar\hat{F}_\pm \tag{1.19}$$

due to equation (1.11). Therewith, one finds

$$\frac{d}{dt}\hat{R}^\dagger\hat{F}_\pm\hat{R} = \frac{s\omega}{i\hbar}\hat{R}^\dagger\left[\hat{F}_\pm, \hat{F}_z\right]\hat{R} = \pm is\omega\hat{R}^\dagger\hat{F}_\pm\hat{R}, \tag{1.20}$$

which, together with

$$\left(\hat{R}^\dagger\hat{F}_\pm\hat{R}\right)\Big|_{t=0} = \hat{F}_\pm, \tag{1.21}$$

implies the formula

$$\hat{R}^\dagger\hat{F}_\pm\hat{R} = e^{\pm is\omega t}\hat{F}_\pm. \tag{1.22}$$

Now, the transformed Hamilton operator is evaluated by inserting the magnetic fields (1.9) and (1.10), the original Hamilton operator (1.12) and the transformation (1.17) into equation (1.16) and using the auxiliary result (1.22):

$$\hat{H}_{\text{rot}} = -s\omega\hat{F}_z + \frac{g_F\mu_B}{\hbar}\hat{R}^\dagger \underbrace{\hat{F}\cdot\left(B_0 + B_1\cos(\omega t)\right)}\hat{R} \tag{1.23}$$

$$\begin{aligned}&= \hat{F}_z\left(b_0 + b_1\cos(\vartheta)\cos(\omega t)\right)\\ &+\tfrac{b_1}{2}\sin(\vartheta)\cos(\omega t)\left(\hat{F}_+e^{-i\varphi} + \hat{F}_-e^{i\varphi}\right)\end{aligned}$$

$$= \hat{F}_z\left(-s\omega + \frac{g_F\mu_B}{\hbar}\left(b_0 + b_1\cos(\vartheta)\cos(\omega t)\right)\right) \tag{1.24}$$

$$+\frac{b_1}{4}\sin(\vartheta)\left(\hat{F}_+e^{i\left((s+1)\omega t+\varphi\right)} + \hat{F}_+e^{i\left((s-1)\omega t+\varphi\right)} + \hat{F}_-e^{-i\left((s+1)\omega t+\varphi\right)} + \hat{F}_-e^{-i\left((s-1)\omega t+\varphi\right)}\right). \tag{1.25}$$

Irrespective of s, two of the last terms are independent of time, while the other two oscillate at a frequency 2ω. It is now assumed, that the time dependent additive contibutions of $\hat{H}_{\text{rot}}$ can be neglected, as they approximately cancel out when a time average over the period $\frac{2\pi}{\omega}$ is performed. This is known as the rotating wave approximation. The Hamilton operator consequently reduces to

$$\hat{H}_{\text{rot}} \approx \left(-s\omega + \frac{g_F\mu_B}{\hbar}b_0\right)\cdot\hat{F}_z + \frac{g_F\mu_B}{\hbar}\frac{b_1\sin(\vartheta)}{2}\left(\hat{F}_x\cos(\varphi) + \hat{F}_y\sin(\varphi)\right) \tag{1.26}$$

$$= \frac{g_F\mu_B}{\hbar}\hat{F}\cdot\underbrace{\begin{pmatrix}\frac{b_1}{2}\sin(\vartheta)\cos(\varphi)\\ \frac{b_1}{2}\sin(\vartheta)\sin(\varphi)\\ b_0 - \frac{\hbar\omega}{|g_F|\mu_B}\end{pmatrix}}_{B_{\text{eff}}}. \tag{1.27}$$

The rotating wave approximation leads to an effective time independent Hamilton operator, which is equivalent to that of the atom sitting in the static magnetic field B_{eff}, which depends on the amplitudes (b_0 and b_1) and on the relative orientation (φ and ϑ) of the original fields, as well as on the radio frequency ω. The key difference between an initially static field and an effective static field is that the effective magnetic field is not governed by the restrictive Maxwell equations. The effective magnetic field is expressed as

$$B_{\text{eff}} = \frac{\hbar\Omega}{g_F\mu_B}\begin{pmatrix}\sin(\theta)\cos(\phi)\\ \sin(\theta)\sin(\phi)\\ \cos(\theta)\end{pmatrix} \tag{1.28}$$

where the generalized Rabi frequency

$$\Omega \equiv \frac{g_F \mu_\mathrm{B}}{\hbar} \sqrt{\left(b_0 - \frac{\hbar \omega}{|g_F| \mu_\mathrm{B}} \right)^2 + \left(\frac{b_1 \sin(\vartheta)}{2} \right)^2} \tag{1.29}$$

and the angle

$$\theta \equiv \arccos\left(\frac{\omega - \frac{|g_F| \mu_\mathrm{B}}{\hbar} b_0}{\Omega} \right) + \frac{s-1}{2} \pi \tag{1.30}$$

are introduced. Similar to the auxiliary result (1.22), one can show, that the projection of $\hat{F}$ in the direction of B_eff (which is essentially the generator of rotations around the axis defined by B_eff) is related to $\hat{F}_z$ by the rotation

$$\hat{R}' \equiv e^{\frac{\varphi \hat{F}_z}{i\hbar}} e^{\frac{\theta \hat{F}_y}{i\hbar}} \tag{1.31}$$

like

$$\hat{R}'^\dagger \hat{F} \cdot \begin{pmatrix} \sin(\theta)\cos(\phi) \\ \sin(\theta)\sin(\phi) \\ \cos(\theta) \end{pmatrix} \hat{R}' = \hat{F}_z. \tag{1.32}$$

This result becomes useful by regarding the rotated state

$$|\psi(\bullet)\rangle'_\mathrm{rot} \equiv \hat{R}' |\psi(\bullet)\rangle_\mathrm{rot}, \tag{1.33}$$

which then fulfills the Schrödinger equation

$$i\hbar \frac{d}{dt} |\psi(t)\rangle'_\mathrm{rot} = \hat{H}'_\mathrm{rot} |\psi(t)\rangle'_\mathrm{rot} \tag{1.34}$$

due to (1.15), where the Hamilton operator $\hat{H}'_\mathrm{rot}$ reads

$$\hat{H}'_\mathrm{rot} = \hat{R}' \hat{H}_\mathrm{rot} \hat{R}'^\dagger = \Omega \hat{F}_z \tag{1.35}$$

due to the auxiliary result (1.22). The solutions to the eigenvalue problem of $\hat{H}'_\mathrm{rot}$ are therefore simply given by the usual spin states $|m\rangle$, i.e.

$$\hat{H}'_\mathrm{rot} |m\rangle = m\hbar\Omega |m\rangle, \tag{1.36}$$

with $m \in \{-F, F\}$ denoting the magnetic quantum number and $F \in \frac{\mathbb{N}}{2}$ denoting the azimuthal quantum number, which is set by the atomic species used in the experiment. With these eigenstates, the solutions to the original Schrödinger equation are approximately retrieved. One finally gets

$$|\psi_m(t)\rangle \equiv \hat{R} \hat{R}'^\dagger e^{\frac{m\Omega t}{i}} |m\rangle \tag{1.37}$$

with

$$i\hbar \frac{d}{dt} |\psi_m(t)\rangle \approx \hat{H} |\psi_m(t)\rangle \approx m\hbar\Omega |\psi_m(t)\rangle. \tag{1.38}$$

Now, the spatial dependency of the fields is introduced. It is assumed that the atomic wavefunctions are both localized enough to perceive the magnetic fields as almost uniform and slow enough to adiabatically follow the state $|\psi_m\rangle$. An atom in the state $|\psi_m\rangle$ then experiences the trapping potential $m\hbar\Omega$, with Ω depending on the position of the atom. By choosing an appropriate conventional magnetic trap (e.g. a quadrupole trap or an Ioffe-Pritchard trap) and a suitable superposed radio frequency field, the atoms are typically confined to the surface of an ellipsoid with a harmonic potential in the direction transverse to that surface.

1.3 Outline of thesis

In terms of broad structure, the thesis is split about evenly into a main body and a collection of appendices. The main body is subdivided into three sections, starting with the construction of the quantum statistical model (in section 2), followed by a derivation of the consequent fundamental equations for classical thermodynamics (in section 3) and finally some thermodynamic calculations (in section 4). These main sections are designed to be comprehensible as a stand alone. They represent a "standard" physicist's approach to a quantum statistical investigation. In contrast, the appendices provide an in depth introduction of some of the utilized "non-standard" mathematical structures and are to be regarded as an equally valuable part of the thesis. Here, "non-standard" means, that some of the heuristic techniques used by physicists for the sake of efficiency are given a more rigorous mathematical basis and notation.

In section 2, the fundamental quantum statistical model for the ultracold Bose gas is constructed. Second quantized Schrödinger field theory is introduced as the appropriate microscopic model and the formalism for the inclusion of trapping is discussed briefly. The considerations on differential geometry are outsourced to appendix C, where integration and differentiation on manifolds is discussed. Then the statistical framework of ensemble theory is presented, introducing the specific types of ensembles used in this thesis. A deeper analysis of the statistical aspects is provided by appendix A, where concepts from probability theory are used to describe entropy and its extremization. The microscopic and the statistical model are then combined in the quantum statistical formalism.

Section 3 provides the link between the quantum statistical model and classical thermodynamics, by finding a simplified expression for the (extended) grand-canonical potential. A grand-canonical description on an arbitrary manifold is considered first and then adapted by extending the grand-canonical description to include superfluidity while restricting the trapping geometry to a two- and three-dimensional box. The simplification of the grand-canonical potential utilizes a result from scattering therory, which is derived in appendix D, where the two-particle system corresponding to the second quantized model from section 2 is analyzed. Ultraviolet divergencies arise in the calculations and are removed via regularization. In appendix E, the source of the divergencies is identified and an original mathematically rigorous alternative to the heuristic regularization scheme is presented.

In section 4, classical thermodynamic calculations are carried out. As an example for a gas on a nontrivial manifold, the thermodynamics of a non-interacting gas on the surface of a sphere is investigated. As an example for a description that includes superfluidity, a two-dimensional box with periodic boundary conditions is treated briefly.

A visual representation of the thesis structure is provided by figure 1.

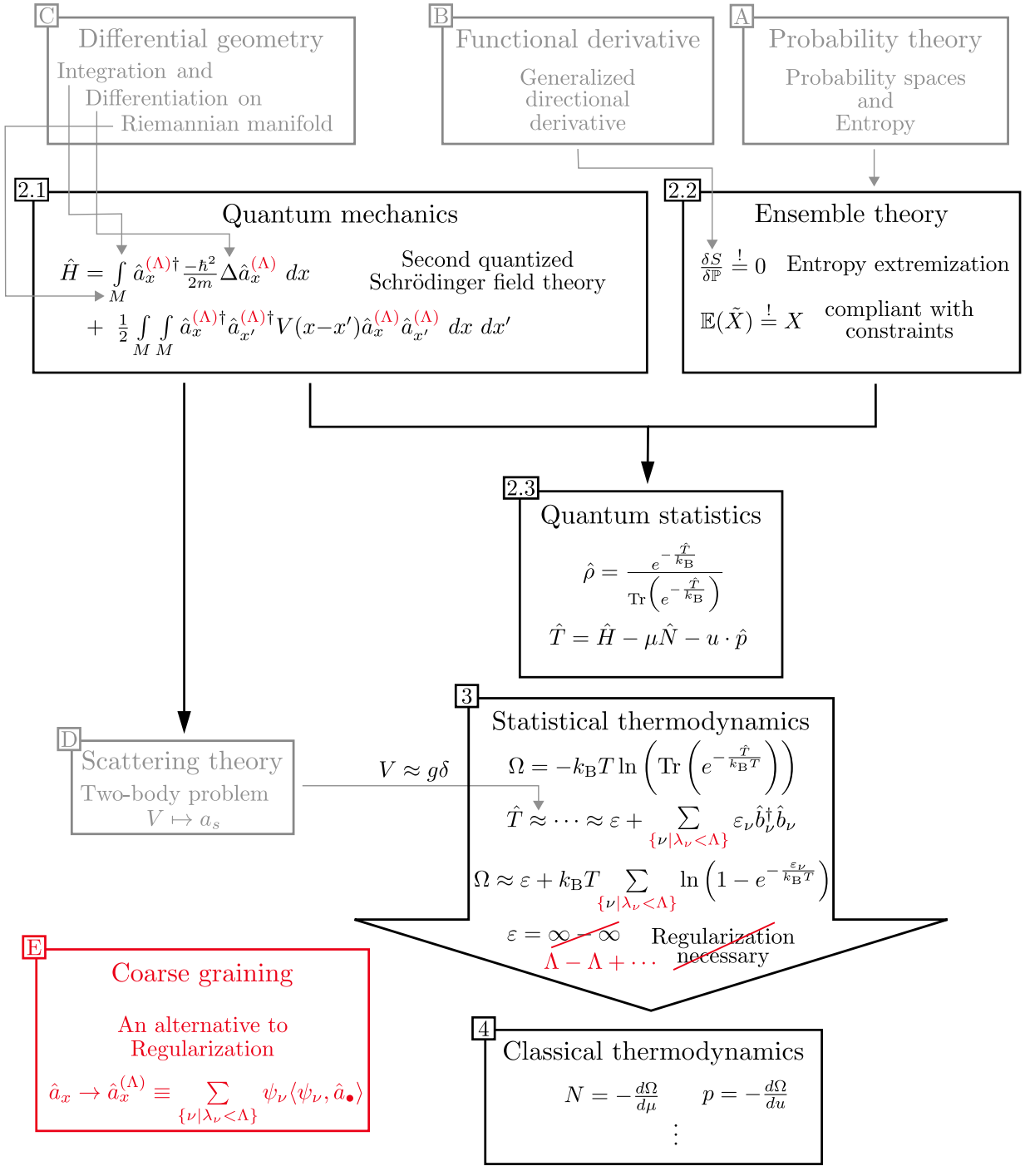


Figure 1: Diagrammatic overview of the nonlinear structure of this thesis. Each block represents the section indicated by the index in its upper left corner. The main body of the thesis is colored black, wheras the various appendices are colored grey (or red). The color red indicates the changes to the usual equations, when coarse graining is applied to avoid divergencies. Contributions of one section to another are indicated by arrows.

2 Modeling

2.1 Quantum mechanics

The constituents of the gas are modeled as identical massive particles. Any internal structure that might be present in non-elementary particles (e.g. atoms) is neglected. Likewise, the non-relativistic limit is assumed to hold. Both of these approximations are justified by the ultracoldness of the gas. In other words: It is assumed that so little energy is thermally distributed in the system, that only a negligible fraction of the particles have enough energy to be internally excited or to move at velocities on the order of the speed of light. Hence, the proper particle number independent microscopic description of this system is second quantized Schrödinger field theory. In this framework, the possible states of the system are given by paths $\left|\Psi(\cdot)\right\rangle$ in a Hilbert space $\mathcal{H}$, that fulfill the Schrödinger equation

$$i\hbar\frac{d}{dt}\left|\Psi(t)\right\rangle = \hat{H}\left|\Psi(t)\right\rangle, \tag{2.1}$$

where the Hamilton operator reads

$$\hat{H} = \int\limits_M \hat{a}_x^\dagger \left(-\frac{\hbar^2}{2m}\Delta\right)\hat{a}_x \; dx + \frac{1}{2}\int\limits_M\int\limits_M \hat{a}_x^\dagger \hat{a}_{x'}^\dagger V(x-x')\hat{a}_x\hat{a}_{x'} \; dx \; dx'. \tag{2.2}$$

From left to right, its two additive components are the non-relativistic kinetic contribution and the contribution of pairwise interaction. The notation is detailed out in the following.

In experimental setups, the gas is always spatially confined via some external trapping potential experienced by each individual particle. A strict confinement to an open region $M \subset \mathbb{R}^3$ corresponds to the limit of the trapping potential going to zero on M and to infinity outside. Trapping the particles on a lower-dimensional submanifold then corresponds to the additional limit of an infinitely tight trapping in all directions locally perpendicular to the manifold. Though neither of these two limits can be reached precisely in the experiment, they are included in the model as a necessary simplification. Depending on the specific limit taken to get to an infinitely tight transverse confinement, the description of the gas on the manifold may be spoiled in the form of a residual potential. To give an example, in [13, eq. (28)], the transversal confinement was chosen constant everywhere on the manifold, resulting in a residual potential dependent on the local curvature. Here, it is assumed that the residual potential vanishes. In the mathematical model, the confinement to a smooth sub manifold M of $\mathbb{R}^3$ is incorporated by setting the co-domain of ladder operators $\hat{a}_\bullet$ to M. (In this thesis, especially the surface of a sphere and the two-dimensional box are investigated in more detail). An explanation of the integration $\int\limits_M dx$ over the manifold M and of the Laplace-Beltrami differential operator is outsourced to appendix C.

As the particles under consideration are assumed to be bosons, the fields of the first quantized formalism take values in $\mathbb{C}$, (as opposed to the fermionic case, where the fields take values in the Grassmann numbers). From canonical quantization follow the according commutation relations for the ladder operators:

$$[\hat{a}_x, \hat{a}_{x'}^\dagger] = \delta(x-x')$$
$$[\hat{a}_x, \hat{a}_{x'}] = 0.$$

The limits necessary for a strict confinement to a submanifold would also entail Dirichlet boundary conditions for the ladder operators $\hat{a}_\bullet$, i.e. $\hat{a}|_{\partial M} = 0$. However, none of the upcoming calculations rely on this specific boundary condition and more general boundary conditions are allowed for, e.g. periodic boundary conditions are used in the treatment of the gas in a box.

$V : \mathbb{R}^3 \to \mathbb{R}$ represents a general two particle interaction potential. As Schrödinger field theory is the nonrelativistic limit of Klein Gordon theory, it also inherits the nonrelativistic limit of Lorentz invariance, that is, invariance under Gallilei transformations. This would imply, that the interaction potential V may only depend on the norm of the distance vector. However, allowing for the more general case of V depending on the distance vector itself can be useful to account for external fields; e.g. a homogenous external magnetic field might align dipolar atoms such that they experience the unisotropic dipole-dipole interaction, see [14].

2.2 Ensemble theory

In experimental setups with high particle numbers, it is neither possible to prepare nor to measure the exact microstate of the system. Additional uncertainty comes through interaction with the surroundings which can't be eliminated completely and is even desired sometimes. The fundamental mathematical construct for including such uncertainty is the probability space. Essentially, it contains a set of all possible microstates of the system and a function (probability measure), that assigns to certain subsets of the possible microstates the probability that the system occupies a state in that subset.

The concept of ensemble theory is a prescription of how to choose the "correct" one among the plethora of possible probability distributions. The first prescription is, that the probability measure must extremize the entropy of the probability space, which is called equilibrium. The interpretation here is, that the probabilities are such that the expected surprisal of a measurement is maximal. The second prescription is, that the extremization may be performed compliant with certain constraints, which models the ability to excert some control over the system in the experiment. More specifically, constraints arising from the experimental setup are mathematically modeled by fixing the expectation values of according random variables. The extremization compliant with these constraints can be performed by introducing Lagrange multipliers. The fixed expectation values and the according Lagrange multipliers are called the thermodynamic variables of the system. The thermodynamic variables relevant in this thesis and their interconnections are listed in table 1.

thermodynamic variable	constraint	Lagrange multiplier	thermodynamic variable
$E \widehat{=}$ inner energy	$\mathbb{E}(\tilde{E}) \stackrel{!}{=} E$	$-\frac{1}{T}$	$T \widehat{=}$temperature
$N \widehat{=}$ particle number	$\mathbb{E}(\tilde{N}) \stackrel{!}{=} N$	$-\frac{\mu}{T}$	$\mu \widehat{=}$chemical potential
$p \widehat{=}$ momentum	$\mathbb{E}(\tilde{p}) \stackrel{!}{=} p$	$-\frac{u}{T}$	$u \widehat{=}$ superfluid velocity

Table 1: Constraints for the extremization of the entropy are given in the form of fixing expectation values $\mathbb{E}(\tilde{X}) \stackrel{!}{=} X$ of random variables $\tilde{X}$ corresponding to certain physical quantities X. The constraints relevant in this thesis are listed alongside the corresponding Lagrange multipliers.

The foundational role of the concept of entropy is in stark contrast to its meager understanding by many physicists. Therefore, in appendix A, entropy is introduced in a constructive and intuitive manner. Its extremization generally involves using a functional derivative, a concept that is introduced in appendix B.

Ensembles obeying special combinations of constraints are given their own names. Table 2 lists the three most commonly used combinations, known as the micro-canonical, the canonical and the grand-canonical ensemble. Additionally, a fourth combination relevant to this thesis is listed, which was given its own original name – the super-canonical ensemble – as it constitutes an extension to the grand-canonical ensemble. The additional constraint of fixing the expectation value of the momentum of the system models superfluidity. This approach constitues an alternative to the usual procedure of introducing superfluidity by switching to a moving reference frame.

label	energy	particle number	momentum
micro-canonical		$\mathbb{E}(\tilde{N}) \stackrel{!}{=} N \wedge \mathrm{Var}(\tilde{N}) \stackrel{!}{=} 0$	
canonical	$\mathbb{E}(\tilde{E}) \stackrel{!}{=} E$	$\mathbb{E}(\tilde{N}) \stackrel{!}{=} N \wedge \mathrm{Var}(\tilde{N}) \stackrel{!}{=} 0$	
grand-canonical	$\mathbb{E}(\tilde{E}) \stackrel{!}{=} E$	$\mathbb{E}(\tilde{N}) \stackrel{!}{=} N$	
super-canonical	$\mathbb{E}(\tilde{E}) \stackrel{!}{=} E$	$\mathbb{E}(\tilde{N}) \stackrel{!}{=} N$	$\mathbb{E}(\tilde{p}) \stackrel{!}{=} p$

Table 2: Labelling of ensembles compliant with special combinations of constraints. The table is to be read as follows: $\mathbb{E}(\tilde{X}) \stackrel{!}{=} X$ means that the expectation value of $\tilde{X}$ is fixed, yet the value of $\tilde{X}(\nu)$ for any particular microstate ν may differ from that expectation value. In contrast, $\mathrm{Var}(\tilde{X}) \equiv \mathbb{E}(\tilde{X}^2) - \mathbb{E}(\tilde{X})^2 = 0$ means that only microstates ν with $\tilde{X}(\nu) = \mathbb{E}(\tilde{X})$ may have non-zero probability.

In this thesis, only the grand-canonical and the super-canonical ensemble are investigated. It should be mentioned, that in experimental setups with photon BECs, the particle number may fluctuate over time, whereas in atomic gases, the particle number is usually fixed, corresponding to the constraint

$\mathrm{Var}(\tilde{N}) \stackrel{!}{=} 0$. It is a usual practice to neglect this constraint to simplify calculations, which is emulated in this thesis as well.

2.3 Quantum statistics

Quantum statistics is the application of ensemble theory to systems whose microstates are described by quantum mechanics. It combines the microscopic with the statistical description of the sytem. In the setup of this thesis, for the statistical description, a grand- or super- canonical ensemble is employed, see section 2.2. The microscopic model on the other hand is second quantized Schrödinger field theory, see section 2.1. In the corresponding quantum statistical framework, one considers a probability space with the sample space being a Schauder basis $\{|\nu\rangle\}$ of the Hilbert space $\mathcal{H}$ and a probability measure $\mathbb{P}$ given by a density operator ρ, as shown in table 3.

probabilty measure	$\mathbb{P}$	$\mathbb{P}(\{\|\nu\rangle\}) = \langle\nu\|\hat{\rho}\|\nu\rangle$	$\hat{\rho}$	density operator
random variable	$\tilde{X}$	$\tilde{X}(\|\nu\rangle) = \left\langle \nu \middle\| \hat{X} \middle\| \nu \right\rangle$	$\hat{X}$	operator
expectation value	$\mathbb{E}$	$\mathbb{E}(\tilde{X}) = \mathrm{Tr}(\hat{X}\hat{\rho})$		

Table 3: One to one correspondence of mathematical and physical notation of quantum statistics.

More precisely, due to ensemble theory (detailed out in the end of appendix A), the density operator takes the shape

$$\hat{\rho} = \frac{1}{Z} e^{-\frac{\hat{T}}{k_\mathrm{B}T}}, \tag{2.3}$$

where the partition function

$$Z = \mathrm{Tr}\left(e^{-\frac{\hat{T}}{k_\mathrm{B}T}}\right) \tag{2.4}$$

and the thermal energy operator

$$\begin{aligned} \hat{T} &\equiv \hat{H} - \mu\hat{N} - u\cdot\hat{p} \\ &= \int\limits_M \hat{a}_x^\dagger \left(-\frac{\hbar^2}{2m}\Delta - i\hbar u\cdot\nabla - \mu\right)\hat{a}_x \, dx + \frac{1}{2}\int\limits_M\int\limits_M \hat{a}_x^\dagger \hat{a}_{x'}^\dagger V(x,x')\hat{a}_x\hat{a}_{x'} \, dx \, dx' \end{aligned} \tag{2.5}$$

are introduced. The particle number operator and the momentum operator are denoted by $\hat{N} = \int\limits_M \hat{a}_x^\dagger\hat{a}_x \, dx$ and $\hat{p} = -i\hbar\int\limits_M \hat{a}_x^\dagger\nabla\hat{a}_x \, dx$, respectively. In case of the grand-canonical description u has to be set to zero, (corresponding to the absence of the constraint of a fixed expecation value of the momentum opeator for the entropy extremization). Foresightedly, one defines the super-/grand-canonical potential

$$\Omega = -k_\mathrm{B}T\ln(Z), \tag{2.6}$$

which plays a major role in the upcoming calculations.

3 Statistical thermodynamics

Bridging the gap between the quantum statistical model and classical thermodynamics requires deriving an analytically and computationally "easy" expression for the functional interdependence of the thermodynamic variables. The grand-/super-canonical potential (2.6) is the prominent candidate as it provides fairly simple access to the thermodynamic variables through simple derivatives as well as to the extremized entropy (as is derived in appendix A). The expression provided by the modeling discussed so far in section 2 is fairly convoluted, though, including in particular the trace of an operator exponential on an infinite dimensional vectorspace (in the partition function (2.4)), as well as multidimensional integrals of operator-valued functions on a manifold (in the thermal energy operator (2.5)).

Evaluation of grand-/super-canonical potential The general procedure adopted in this section to find a simplified expression for Ω is layed out: The trace in the partition function (2.4) is independent of the choice of the basis and can be calculated most easily when the chosen basis is orthonormal and composed of eigenvectors of the operator exponential it is taken of. Constructing such a basis involves inserting a range of transformations of the ladder operators $\hat{a}_x$ and additional approximations into the thermal energy operator to mold it into the shape

$$\hat{T} \approx \varepsilon + \sum_{\nu} \varepsilon_\nu \hat{b}_\nu^\dagger \hat{b}_\nu, \tag{3.1}$$

where the summation over ν then runs over some countable set. (A technical requirement for this step is knowing the solutions to the eigenvalue problem of the Laplace-Beltrami operator). If the transformations of the ladder operators lead to bosonic commutation relations for $\hat{b}_\nu$, then the corresponding Fockstates $|n_0 \cdots\rangle \equiv \sum_{\nu} \frac{\left(\hat{b}_\nu^\dagger\right)^{n_\nu}}{\sqrt{n_\nu!}} |0\rangle$ (for any sequence $(n_\nu)_{\nu\in\mathbb{N}}$ in $\mathbb{N}$ with $\sum_\nu n_\nu < \infty$) form an orthonormal Schauder basis, suitable for calculating the trace:

$$\begin{aligned}
Z &= \mathrm{Tr}\left(e^{-\frac{\hat{T}}{k_\mathrm{B}T}}\right) \\
&= \sum_{\substack{(n_\nu)_{\nu\in\mathbb{N}} \\ \sum_\nu n_\nu < \infty}} \left\langle n_0 \cdots \middle| e^{-\frac{\varepsilon + \sum_{\nu\in\mathbb{N}} \varepsilon_\nu \hat{b}_\nu^\dagger \hat{b}_\nu}{k_\mathrm{B}T}} \middle| n_0 \cdots \right\rangle \\
&= e^{-\frac{\varepsilon}{k_\mathrm{B}T}} \sum_{\substack{(n_\nu)_{\nu\in\mathbb{N}} \\ \sum_\nu n_\nu < \infty}} e^{-\frac{\sum_{\nu\in\mathbb{N}} \varepsilon_\nu n_\nu}{k_\mathrm{B}T}} \\
&= e^{-\frac{\varepsilon}{k_\mathrm{B}T}} \sum_{\substack{(n_\nu)_{\nu\in\mathbb{N}} \\ \sum_\nu n_\nu < \infty}} \prod_{\nu\in\mathbb{N}} \left(e^{-\frac{\varepsilon_\nu}{k_\mathrm{B}T}}\right)^{n_\nu} \\
&= e^{-\frac{\varepsilon}{k_\mathrm{B}T}} \prod_{\nu\in\mathbb{N}} \sum_{n_\nu\in\mathbb{N}} \left(e^{-\frac{\varepsilon_\nu}{k_\mathrm{B}T}}\right)^{n_\nu} \\
&= e^{-\frac{\varepsilon}{k_\mathrm{B}T}} \prod_{\nu\in\mathbb{N}} \frac{1}{1 - e^{-\frac{\varepsilon_\nu}{k_\mathrm{B}T}}}
\end{aligned} \tag{3.2}$$

It is important to note, that the convergence of the geometric series in the last equality implies restrictions for the thermodynamic variables T, μ and u. By convention of sign, the temperature has to be non-negative, while the energies ε_ν, which depend on both μ and u, must be positive. One ends up with the simple expression

$$\begin{aligned}
\Omega &= -k_\mathrm{B}T \ln(Z) \\
&= \varepsilon + k_\mathrm{B}T \sum_{\nu} \ln\left(1 - e^{-\frac{\varepsilon_\nu}{k_\mathrm{B}T}}\right)
\end{aligned} \tag{3.3}$$

for the grand-/super-canonical potential, composed only of elementary mathematical expressions, apart from a series and the complexity hidden in ε and ε_ν.

In the following, the simplification of the grand-/super-canonical potential is executed for the case of a grand-canonical ensemble ($u = 0$) and an arbitrary manifold M. Afterwards the procedure is adapted, by extending it to a super-canonical ensemble ($u \in \mathbb{R}$) and simultaneously restricting it to a box $M = [0, L]^n$ with periodic boundary conditions.

First quantized interaction-free description In preparation for the upcoming transformations of the thermal energy operator, it is useful to discuss the microscopic first quantized description of the system, which is governed by the Laplace-Beltrami operator. This linear differential operator is constructed and discussed in appendix C. A complete set of orthonormal solutions to its eigenvalue problem is assumed to be known, compliant with the given boundary conditions. More precisely, a countable set of functions $\psi_\nu : M \to \mathbb{C}$ and a set of corresponding scalars $e_\nu \in [0, \infty[$ are assumed to be known, that fulfill the differential equation

$$-\frac{\hbar^2}{2m}\Delta\psi_\nu = e_\nu\psi_\nu \tag{3.4}$$

while respecting the boundary conditions on $\psi|_{\partial M}$. Furthermore, without loss of generality, they are assumed to be orthonormal

$$\langle\psi_\nu \mid \psi_\kappa\rangle = \delta_{\nu\kappa} \tag{3.5}$$

with respect to the scalar product

$$\langle\psi \mid \phi\rangle \equiv \int_M \psi^*(x)\phi(x)\ dx \tag{3.6}$$

and to form a Schauder basis of the vectorspace $\mathcal{H}_1$ of the first quantized microscopic theory. Thus, any function $\phi \in \mathcal{H}_1$ is expressible as a linear combination

$$\phi = \sum_\nu \langle\psi_\nu \mid \phi\rangle\psi_\nu \tag{3.7}$$

of the basis elements.

The Laplace-Beltrami operator has the property of commuting with the operation of taking the real part pointwise, i.e. $\mathfrak{Re}(\Delta\phi) = \Delta\mathfrak{Re}(\phi)$. Due to linearity, it also commutes with taking the imaginary part and with complex conjugation. Consequently, ψ_ν^* is in the same eigenspace as ψ_ν. Therefore, without loss of generality, it is assumed that the complex conjugate of any eigenfunction is also an element of the basis; i.e. for each index ν exists an index ν^*, such that

$$\psi_\nu^* = \psi_{\nu^*}. \tag{3.8}$$

This assumption may contradict exotic boundary conditions, but at least the common cases of periodic and Dirichlet boundary conditions are invariant under complex conjugation.

3.1 Grand-canonical description on an arbitrary manifold

A grand-canonical ensemble of an interacting gas on an arbitrary manifold M is considered. By setting u to zero in the general expression (2.5) for the thermal energy operator, one gets

$$\hat{T} = \int_M \hat{a}_x^\dagger \left(-\frac{\hbar^2}{2m}\Delta - \mu\right)\hat{a}_x\ dx + \frac{1}{2}\int_M\int_M \hat{a}_x^\dagger\hat{a}_{x'}^\dagger V(x-x')\hat{a}_x\hat{a}_{x'}\ dx\ dx', \tag{3.9}$$

which is molded into the desired shape (3.1) in the following.

3.1.1 Simplifying the thermal energy operator

Kinetic contribution The first step of transforming the thermal energy operator is getting rid of the Laplace-Beltrami differential operator in the kinetic contribution. To this end, using (3.7), the spatially dependent function $\hat{a}_\bullet$ of ladder operators is expanded into a linear combination of the eigenfunctions of the Laplace Beltrami operator like

$$\hat{a}_x = \sum_\nu \hat{b}_\nu \psi_\nu(x), \tag{3.10}$$

with operator valued coefficients

$$\hat{b}_\nu \equiv \int\limits_M \psi^*_\nu(x)\hat{a}_x \; dx. \tag{3.11}$$

The new ladder operators $\hat{b}_\nu$ inherit the discrete version

$$\left[\hat{b}_\kappa, \hat{b}^\dagger_\nu\right] = \int\limits_M \int\limits_M \psi^*_\kappa(x)\psi_\nu(x') \left[\hat{a}_x, \hat{a}^\dagger_{x'}\right] \; dx \; dx' = \int\limits_M \psi^*_\kappa(x)\psi_\nu(x) \; dx = \delta_{\kappa\nu} \tag{3.12}$$

$$\left[\hat{b}_\kappa, \hat{b}_{\kappa'}\right] = \int\limits_M \int\limits_M \psi^*_{\nu'}(x)\psi^*_\nu(x') \left[\hat{a}_x, \hat{a}_{x'}\right] \; dx \; dx' = 0 \tag{3.13}$$

of the bosonic commutation relations (2.1) of the operators $\hat{a}_x$. Inserting this transformation of the ladder operators into the thermal energy operator, yields

$$\begin{aligned}\hat{T} = &\sum_{\nu,\kappa} \hat{b}^\dagger_\nu \hat{b}_\kappa \underbrace{\int\limits_M \psi^*_\nu(x) \left(-\frac{\hbar^2}{2m}\Delta - \mu\right) \psi_\kappa(x) \; dx}_{=(e_\kappa - \mu)\delta_{\nu\kappa}} \\ &+ \frac{1}{2} \sum_{\nu,\nu',\kappa,\kappa'} \hat{b}^\dagger_\nu \hat{b}^\dagger_{\nu'} \hat{b}_\kappa \hat{b}_{\kappa'} \int\limits_M \int\limits_M \psi^*_\nu(x)\psi^*_{\nu'}(x) V(x-x') \psi_\kappa(x)\psi_{\kappa'}(x) \; dx \; dx'\end{aligned} \tag{3.14}$$

As a small digression, one may consider the non-interacting case (where $V = 0$). Then, with the identification $\varepsilon = 0$ and $\varepsilon_\nu = e_\nu - \mu$, the thermal energy operator (3.14) is already of the desired quadratic and diagonal shape (3.1), such that the grand-canonical potential (3.3) evaluates to

$$\Omega = k_\mathrm{B} T \sum_\nu \ln(1 - e^{-\frac{e_k - \mu}{k_\mathrm{B} T}}). \tag{3.15}$$

Quartic to quadratic This expression for the thermal energy operator contains products of up to four ladder operators. In order to reduce this number to two one first makes the ansatz

$$\hat{b}_0 \overset{!}{\approx} \sqrt{N_0}, \tag{3.16}$$

where $N_0 \in [0, \infty[$ is a dimensionless variational parameter, the value of which is yet to be determined. Within the bounds of this approximation, the number operator $\hat{b}^\dagger_0 \hat{b}_0$ for the occupation of the groundstate is equal to N_0. Consequently, the variational parameter N_0 is interpreted as an approximation of the expectation value of the ground state occupation number. Here, by choice, the index $\nu = 0$ corresponds to the lowest energy $e_0 = \min\limits_\nu e_\nu$. With this approximation, the thermal energy operator is decomposed into five additive contributions $\hat{T}_i$, each containig only products of $i \in \{0, \cdots, 4\}$ ladder operators, respectively:

$$\hat{T} \approx \sum_{i=0}^4 \hat{T}_i. \tag{3.17}$$

The summation in the interaction term of $\hat{T}$ runs over the set Q of all tuples $(\nu, \nu'\kappa, \kappa')$ of four quantum numbers. The set

$$Q = \bigcup_{i=0}^4 Q_i \tag{3.18}$$

is partitioned into five sets

$$Q_i \equiv \left\{(\nu,\nu'\kappa,\kappa')\middle| 4-\delta_{\nu 0}-\delta_{\nu' 0}-\delta_{\kappa 0}-\delta_{\kappa' 0}=i\right\} \tag{3.19}$$

sorted by the number of non-zero quantum numbers. Each set Q_i comprises exactly all those tuples, that correspond to a product of i ladder operators; they read

$$\begin{aligned}
Q_0 =&\{(0,0,0,0)\} \\
Q_1 =&\{(\nu,0,0,0)|\nu\neq 0\} \\
&\cup\{(0,\nu',0,0)|\nu'\neq 0\} \\
&\cup\{(0,0,\kappa,0)|\kappa\neq 0\} \\
&\cup\{(0,0,0,\kappa')|\kappa'\neq 0\} \\
Q_2 =&\{(\nu,\nu',0,0)|\nu,\nu'\neq 0\} \\
&\cup\{(\nu,0,\kappa,0)|\nu,\kappa\neq 0\} \\
&\cup\{(\nu,0,0,\kappa')|\nu,\kappa'\neq 0\} \\
&\cup\{(0,\nu',\kappa,0)|\nu',\kappa\neq 0\} \\
&\cup\{(0,\nu',0,\kappa')|\nu',\kappa'\neq 0\} \\
&\cup\{(0,0,\kappa,\kappa')|\kappa,\kappa'\neq 0\} \\
Q_3 =&\{(\nu,\nu',\kappa,0)|\nu,\nu',\kappa\neq 0\} \\
&\cup\{(\nu,\nu',0,\kappa')|\nu,\nu',\kappa'\neq 0\} \\
&\cup\{(\nu,0,\kappa,\kappa')|\nu,\kappa,\kappa'\neq 0\} \\
&\cup\{(0,\nu',\kappa,\kappa')|\nu',\kappa,\kappa'\neq 0\} \\
Q_4 =&\{(\nu,\nu',\kappa,\kappa')|\nu,\nu',\kappa,\kappa'\neq 0\}.
\end{aligned}$$

That way, one reads out the first three contributions $\hat{T}_i$ of the thermal energy operator

$$\hat{T}_0 = N_0(e_0-\mu)+\frac{1}{2}N_0^2\int\limits_M\int\limits_M V(x-x')|\psi_0(x)|^2|\psi_0(x')|^2\ dx\ dx' \tag{3.20}$$

$$\begin{aligned}
\hat{T}_1 =&N_0^{\frac{3}{2}}\sum_{\nu\neq 0}\hat{b}_\nu^\dagger\int\limits_M\int\limits_M\frac{V(x-x')+V(x'-x)}{2}\psi_\nu^*(x)\psi_0(x)|\psi_0(x')|^2\ dx\ dx' \\
&+N_0^{\frac{3}{2}}\sum_{\kappa\neq 0}\hat{b}_\kappa\int\limits_M\int\limits_M\frac{V(x-x')+V(x'-x)}{2}\psi_0^*(x)\psi_\kappa(x)|\psi_0(x')|^2\ dx\ dx'
\end{aligned} \tag{3.21}$$

$$\begin{aligned}
\hat{T}_2 =&\sum_{\nu\neq 0}\hat{b}_\nu^\dagger\hat{b}_\nu(e_\nu-\mu) \\
&+N_0\sum_{\nu,\nu'\neq 0}\hat{b}_\nu^\dagger\hat{b}_{\nu'}^\dagger\int\limits_M\int\limits_M\frac{V(x-x')}{2}\psi_\nu^*(x)\psi_{\nu'}^*(x')\psi_0(x)\psi_0(x')\ dx\ dx' \\
&+N_0\sum_{\kappa,\kappa'\neq 0}\hat{b}_\kappa\hat{b}_{\kappa'}\int\limits_M\int\limits_M\frac{V(x-x')}{2}\psi_0^*(x)\psi_0^*(x')\psi_\kappa(x)\psi_{\kappa'}(x')\ dx\ dx' \\
&+N_0\sum_{\nu,\kappa\neq 0}\hat{b}_\nu^\dagger\hat{b}_\kappa\int\limits_M\int\limits_M\frac{V(x-x')+V(x'-x)}{2}\psi_\nu^*(x)\psi_0^*(x')\Big(\psi_\kappa(x)\psi_0(x')+\psi_0(x)\psi_\kappa(x')\Big)\ dx\ dx'.
\end{aligned} \tag{3.22}$$

The unwanted contributions $\hat{T}_3$ and $\hat{T}_4$ with higher order operator products are now discarded:

$$\hat{T}\overset{!}{\approx}\hat{T}_0+\hat{T}_1+\hat{T}_2 \tag{3.23}$$

This crude approximation is later attenuated by the optimal choice of the variational parameter N_0.

Coefficients Next, the coefficients of the operators in $\hat{T}_0$, $\hat{T}_1$ and $\hat{T}_2$ are simplified, which is demonstrated exemplarily for the coefficient

$$c\equiv\int\limits_M\int\limits_M V(x-x')\psi_\nu^*(x)\psi_{\nu'}^*(x')\psi_0(x)\psi_0(x')\ dx\ dx'. \tag{3.24}$$

The general short-range interaction, given by the two-particle interaction potential V, is approximated by contact-interaction

$$V(x-x')\overset{!}{\approx}g\delta(x-x'), \tag{3.25}$$

where $g\in\mathbb{R}$ denotes the interaction strength. It is necessary to specify, which of the properties of the two-particle interaction potential V ought to be preserved by the choice of the interaction strength g. It is a custom to choose a value for g such that $g\delta$ and V have the same s-wave scattering length. In Appendix

D, which deals with scattering theory, $a_s(\kappa)$ is introduced as a measure for the total scattering capacity of the interaction potential V for an incoming wave with wavenumber κ. Inserting the approximation (3.25) into the coeeficients (3.24), reduces the double integrals to a single integral:

$$c \approx g \int_M \psi_\nu^*(x)\psi_{\nu'}^*(x)\psi_0(x)\psi_0(x)\ dx \tag{3.26}$$

Additionally, the integrands are further simplified by approximating the function ψ_0 by a real positive constant. More precisely, to preserve the normalization $\langle\psi_0, \psi_0\rangle = 1$, the constant has to be chosen as the inverse of the square root of the generalized volume $|M| \equiv \int_M 1\ dx$ of the manifold M, i.e.

$$\psi_0 \overset{!}{\approx} \frac{1}{\sqrt{|M|}}. \tag{3.27}$$

This allows factoring out a pair of plain and/or complex conjugated ψ_0 from the integral, yielding

$$c \approx \frac{g}{|M|}\int_M \psi_\nu^*(x)\psi_{\nu'}^*(x)\ dx = \frac{g}{|M|}\langle\psi_\nu \mid \psi_{\nu'}^*\rangle, \tag{3.28}$$

where the integral was identified with the first quantized scalar product (3.6). Analogous simplifications of the other coefficients are performed and inserted back into the operators $\hat{T}_i$. Evaluating the scalar products with the help of the orthonormality (3.5) and Equation (3.8), one gets

$$\begin{aligned}\hat{T}_0 &= N_0(e_0 - \mu) + \frac{gN_0^2}{2|M|}\langle\psi_0 \mid \psi_0\rangle \\ &= N_0\left(\frac{gN_0}{2|M|} + e_0 - \mu\right)\end{aligned} \tag{3.29}$$

$$\hat{T}_1 = \frac{gN_0^{\frac{3}{2}}}{|M|}\left(\sum_{\nu\neq 0}\hat{b}_\nu^\dagger\langle\psi_\nu \mid \psi_0\rangle + \sum_{\kappa\neq 0}\hat{b}_\kappa\langle\psi_0 \mid \psi_\kappa\rangle\right) = 0 \tag{3.30}$$

$$\begin{aligned}\hat{T}_2 =& \sum_{\nu\neq 0}\hat{b}_\nu^\dagger\hat{b}_\nu(e_\nu - \mu) \\ &+ \frac{gN_0}{2|M|}\left(\sum_{\nu,\nu'\neq 0}\hat{b}_\nu^\dagger\hat{b}_{\nu'}^\dagger\langle\psi_\nu \mid \psi_{\nu'}^*\rangle + \sum_{\kappa,\kappa'\neq 0}\hat{b}_\kappa\hat{b}_{\kappa'}\langle\psi_\kappa^* \mid \psi_{\kappa'}\rangle + 4\sum_{\nu,\kappa\neq 0}\hat{b}_\nu^\dagger\hat{b}_\kappa\langle\psi_\nu \mid \psi_\kappa\rangle\right) \\ =& \sum_{\nu\neq 0}\left(\hat{b}_\nu^\dagger\hat{b}_\nu(e_\nu - \mu) + \frac{gN_0}{2|M|}\left(\hat{b}_\nu^\dagger\hat{b}_{\nu^*}^\dagger + \hat{b}_\nu\hat{b}_{\nu^*} + 4\hat{b}_\nu^\dagger\hat{b}_\nu\right)\right).\end{aligned} \tag{3.31}$$

Adding up these three contributions in (3.23), the thermal energy operator takes the shape

$$\hat{T} \approx N_0\left(\frac{gN_0}{2|M|} + e_0 - \mu\right) + \sum_{\nu\neq 0}\left(\hat{b}_\nu^\dagger\hat{b}_\nu\left(\frac{2gN_0}{|M|} + e_\nu - \mu\right) + \frac{gN_0}{2|M|}\left(\hat{b}_\nu^\dagger\hat{b}_{\nu^*}^\dagger + \hat{b}_\nu\hat{b}_{\nu^*}\right)\right), \tag{3.32}$$

which only contains terms with either zero or two operators.

Diagonalization/Bogoliubov transformation The last step in molding $\hat{T}$ into the shape (3.1) involves eliminating the off-diagonal opertor pairs $\hat{b}_\nu^\dagger\hat{b}_{\nu^*}^\dagger$ and $\hat{b}_\nu\hat{b}_{\nu^*}$. To this end, a second transformation

$$\hat{b}_\nu \equiv v_\nu\hat{B}_\nu + v_\nu'\hat{B}_{\nu^*}^\dagger \tag{3.33}$$

of the ladder operators – called the Bogoliubov transformation – is employed. Combining this equation with its adjoint gives a linear transformation which is inverted by inverting the coefficient matrix:

$$\begin{pmatrix}\hat{b}_\nu \\ \hat{b}_{\nu^*}^\dagger\end{pmatrix} = \begin{pmatrix}v_\nu & v_\nu' \\ v_{\nu^*}'^* & v_{\nu^*}^*\end{pmatrix}\begin{pmatrix}\hat{B}_\nu \\ \hat{B}_{\nu^*}^\dagger\end{pmatrix} \Leftrightarrow \begin{pmatrix}\hat{B}_\nu \\ \hat{B}_{\nu^*}^\dagger\end{pmatrix} = \frac{1}{v_\nu v_{\nu^*}^* - v_\nu' v_{\nu^*}'^*}\begin{pmatrix}v_{\nu^*}^* & -v_\nu' \\ -v_{\nu^*}'^* & v_\nu\end{pmatrix}\begin{pmatrix}\hat{b}_\nu \\ \hat{b}_{\nu^*}^\dagger\end{pmatrix}. \tag{3.34}$$

From the first line one reads out the expression

$$\hat{B}_\nu = \frac{v_{\nu^*}^* \hat{b}_\nu - v_\nu' \hat{b}_{\nu^*}^\dagger}{v_{\nu^*}^* v_\nu - v_\nu' v_{\nu^*}'^*}. \tag{3.35}$$

The correct choice for the complex valued coefficients v_ν and v_ν' is now determined. The ladder operators $\hat{B}_\nu$ must inherit the bosonic commutation relations (3.12) from their predecessors $\hat{b}_\nu$. With the auxiliary calculation

$$\begin{aligned}
&\left[v_{\kappa^*}^* \hat{b}_\kappa - v_\kappa' \hat{b}_{\kappa^*}^\dagger, v_{\nu^*}^* \hat{b}_\nu - v_\nu' \hat{b}_{\nu^*}^\dagger\right] \\
=&v_{\kappa^*}^* v_{\nu^*}^* \left[\hat{b}_\kappa, \hat{b}_\nu\right] - v_{\kappa^*}^* v_\nu' \left[\hat{b}_\kappa, \hat{b}_{\nu^*}^\dagger\right] - v_\kappa' v_{\nu^*}^* \left[\hat{b}_{\kappa^*}^\dagger, \hat{b}_\nu\right] + v_\kappa' v_\nu' \left[\hat{b}_{\kappa^*}^\dagger, \hat{b}_{\nu^*}^\dagger\right] \\
=&v_\kappa' v_{\nu^*}^* \delta_{\kappa^*\nu} - v_{\kappa^*}^* v_\nu' \delta_{\kappa\nu^*} \\
=&0,
\end{aligned} \tag{3.36}$$

the commutator of two annihilation operators

$$\left[\hat{B}_\kappa, \hat{B}_\nu\right] = \frac{1}{v_\kappa v_{\kappa^*}^* - v_\kappa' v_{\kappa^*}'^*} \frac{1}{v_\nu v_{\nu^*}^* - v_\nu' v_{\nu^*}'^*} \left[v_{\kappa^*}^* \hat{b}_\kappa - v_\kappa' \hat{b}_{\kappa^*}^\dagger, v_{\nu^*}^* \hat{b}_\nu - v_\nu' \hat{b}_{\nu^*}^\dagger\right] = 0 \tag{3.37}$$

turns out to be zero irrespective of the choice of the coefficients. In contrast, using the auxiliary calculation

$$\begin{aligned}
&\left[v_{\kappa^*}^* \hat{b}_\kappa - v_\kappa' \hat{b}_{\kappa^*}^\dagger, v_{\nu^*} \hat{b}_\nu^\dagger - v_\nu'^* \hat{b}_{\nu^*}\right] \\
=&v_{\kappa^*}^* v_{\nu^*} \left[\hat{b}_\kappa, \hat{b}_\nu^\dagger\right] - v_{\kappa^*}^* v_\nu'^* \left[\hat{b}_\kappa, \hat{b}_{\nu^*}\right] - v_\kappa' v_{\nu^*} \left[\hat{b}_{\kappa^*}^\dagger, \hat{b}_\nu^\dagger\right] + v_\kappa' v_\nu'^* \left[\hat{b}_{\kappa^*}^\dagger, \hat{b}_{\nu^*}\right] \\
=&v_{\kappa^*}^* v_{\nu^*} \delta_{\kappa\nu} - v_\kappa' v_\nu'^* \delta_{\kappa^*\nu^*} \\
=&\left(v_{\nu^*}^* v_{\nu^*} - v_\nu' v_\nu'^*\right) \delta_{\kappa\nu},
\end{aligned} \tag{3.38}$$

the commutator of an annihilation operator with a creation operator evaluates to

$$\left[\hat{B}_\kappa, \hat{B}_\nu^\dagger\right] = \frac{1}{v_\kappa v_{\kappa^*}^* - v_\kappa' v_{\kappa^*}'^*} \frac{1}{v_\nu^* v_{\nu^*} - v_\nu'^* v_{\nu^*}'} \left[v_{\kappa^*}^* \hat{b}_\kappa - v_\kappa' \hat{b}_{\kappa^*}^\dagger, v_{\nu^*} \hat{b}_\nu^\dagger - v_\nu'^* \hat{b}_{\nu^*}\right] = \frac{|v_{\nu^*}|^2 - |v_\nu'|^2}{|v_\nu^* v_{\nu^*} - v_\nu'^* v_{\nu^*}'|^2} \delta_{\kappa\nu}, \tag{3.39}$$

which entails the condition

$$\frac{|v_{\nu^*}|^2 - |v_\nu'|^2}{|v_\nu^* v_{\nu^*} - v_\nu'^* v_{\nu^*}'|^2} \stackrel{!}{=} 1 \tag{3.40}$$

for the coefficients. The thermal energy operator is now expressed in terms of the new ladder operators $\hat{B}_\nu$. With the Bogoliubov transformation (3.33), the operator pairs in the thermal energy operator evaluate to

$$\begin{aligned}
\hat{b}_\nu^\dagger \hat{b}_\nu = v_\nu v_\nu'^* \hat{B}_\nu \hat{B}_{\nu^*} &+ v_\nu^* v_\nu' \hat{B}_\nu^\dagger \hat{B}_{\nu^*}^\dagger \\
&+ v_\nu' v_\nu'^* \hat{B}_{\nu^*} \hat{B}_{\nu^*}^\dagger \\
&+ v_\nu v_\nu^* \hat{B}_\nu^\dagger \hat{B}_\nu
\end{aligned}
\qquad
\begin{aligned}
\hat{b}_\nu \hat{b}_{\nu^*} = v_\nu v_{\nu^*} \hat{B}_\nu \hat{B}_{\nu^*} &+ v_\nu' v_{\nu^*}' \hat{B}_\nu^\dagger \hat{B}_{\nu^*}^\dagger \\
&+ v_\nu v_{\nu^*}' \hat{B}_\nu \hat{B}_\nu^\dagger \\
&+ v_\nu' v_{\nu^*} \hat{B}_{\nu^*}^\dagger \hat{B}_{\nu^*}
\end{aligned}
\qquad
\begin{aligned}
\hat{b}_\nu \hat{b}_{\nu^*} + \hat{b}_\nu^\dagger \hat{b}_{\nu^*}^\dagger = \left(v_\nu v_{\nu^*} + v_\nu'^* v_{\nu^*}'^*\right) \hat{B}_\nu \hat{B}_{\nu^*} \\
+ \left(v_\nu^* v_{\nu^*}^* + v_\nu' v_{\nu^*}'\right) \hat{B}_\nu^\dagger \hat{B}_{\nu^*}^\dagger \\
+ \left(v_\nu v_{\nu^*}' + v_\nu^* v_{\nu^*}'^*\right) \hat{B}_\nu \hat{B}_\nu^\dagger \\
+ \left(v_\nu' v_{\nu^*} + v_\nu'^* v_{\nu^*}^*\right) \hat{B}_{\nu^*}^\dagger \hat{B}_{\nu^*}.
\end{aligned}$$

Inserting these expressions into (3.32) yields

$$
\begin{aligned}
\hat{T} \approx\ & N_0 \left(\frac{gN_0}{2|M|} + e_0 - \mu \right) \\
& + \sum_{\nu \neq 0} \left(\hat{B}_\nu \hat{B}_{\nu^*} \left(v_\nu v'^*_\nu \left(\frac{2gN_0}{|M|} + e_\nu - \mu \right) + \left(v_\nu v_{\nu^*} + v'^*_\nu v'^*_{\nu^*} \right) \frac{gN_0}{2|M|} \right) \right. \\
& \quad + \hat{B}^\dagger_\nu \hat{B}^\dagger_{\nu^*} \left(v^*_\nu v'_\nu \left(\frac{2gN_0}{|M|} + e_\nu - \mu \right) + \left(v^*_\nu v^*_{\nu^*} + v'_\nu v'_{\nu^*} \right) \frac{gN_0}{2|M|} \right) \\
& \quad + \hat{B}_\nu \hat{B}^\dagger_\nu \left(v'_{\nu^*} v'^*_{\nu^*} \left(\frac{2gN_0}{|M|} + e_\nu - \mu \right) + \left(v_\nu v'_{\nu^*} + v^*_\nu v'^*_{\nu^*} \right) \frac{gN_0}{2|M|} \right) \\
& \quad \left. + \hat{B}^\dagger_\nu \hat{B}_\nu \left(v_\nu v^*_\nu \left(\frac{2gN_0}{|M|} + e_\nu - \mu \right) + \left(v'_\nu v_{\nu^*} + v'^*_\nu v^*_{\nu^*} \right) \frac{gN_0}{2|M|} \right) \right).
\end{aligned} \tag{3.41}
$$

The coefficients of the non-diagonal operator pairs $\hat{B}_\nu \hat{B}_{\nu^*}$ are set to zero:

$$
\left(v^*_\nu v^*_{\nu^*} + v'_\nu v'_{\nu^*} \right) \frac{gN_0}{2|M|} + v^*_\nu v'_\nu \left(\frac{2gN_0}{|M|} + e_\nu - \mu \right) \stackrel{!}{=} 0 \tag{3.42}
$$

One now has four conditions for the coefficients v_ν, v_{ν^*}, v'_ν, and v'_{ν^*}, that sufficiently define them, namely Equations (3.40) and (3.42), as well as the same equations evaluated at the index ν^* instead of ν. After minor algebraic rearrangement, Equation (3.40) and its starred form are condensed into

$$
v^*_{\nu^*} v'_{\nu^*} = v^*_\nu v'_\nu = - \left(4 + 2|M| \frac{e_\nu - \mu}{gN_0} \right)^{-1} \left(v^*_\nu v^*_{\nu^*} + v'_\nu v'_{\nu^*} \right), \tag{3.43}
$$

wheras equation (3.42) and its starred form are merged into

$$
|v_\nu|^2 - |v'_{\nu^*}|^2 = |v_{\nu^*}|^2 - |v'_\nu|^2 = |v^*_\nu v_{\nu^*} - v'^*_\nu v'_{\nu^*}|^2. \tag{3.44}
$$

The first equality of (3.43) is rearranged into

$$
\frac{v^*_{\nu^*}}{v'_\nu} = \frac{v^*_\nu}{v'_{\nu^*}} \tag{3.45}
$$

which gives

$$
-2 \left(2 + |M| \frac{e_\nu - \mu}{gN_0} \right) = \frac{v'_{\nu^*}}{v^*_\nu} + \frac{v^*_\nu}{v'_{\nu^*}}, \tag{3.46}
$$

in conjunction with the second equality of (3.43). As the left hand side of Equation (3.46) is real and since it holds

$$
0 = \Im(z + z^{-1}) = \Im(z) \left(1 + \frac{1}{|z|} \right) \Rightarrow \Im(z) = 0 \tag{3.47}
$$

for any complex number $z \in \mathbb{C} \setminus \{0\}$, one finds

$$
\frac{v'_{\nu^*}}{v^*_\nu} \in \mathbb{R}. \tag{3.48}
$$

Combining the first equality of (3.43) and (3.44) yields

$$
|v_\nu| = |v_{\nu^*}| \quad \wedge \quad |v'_\nu| = |v'_{\nu^*}|, \tag{3.49}
$$

which in turn gives

$$
|v_\nu|^2 - |v'_\nu|^2 = 1 \tag{3.50}
$$

upon insertion into the second equality of (3.44). The set of equations (3.45), (3.46), (3.49) and (3.50) is equivalent to the original set of conditions (3.43) and (3.44). The new set of conditions is evidently invariant under the simultaneous transformation

$$\begin{aligned} v_\nu &\to e^{i\alpha} v_\nu & v'_\nu &\to e^{i\alpha'} v'_{\nu^*} \\ v_{\nu^*} &\to e^{-i\alpha'} v_{\nu^*} & v'_{\nu^*} &\to e^{-i\alpha} v'_{\nu^*} \end{aligned} \tag{3.51}$$

of all coefficients, for any two angles $\alpha, \alpha' \in \mathbb{R}$. Hence, one has the freedom to choose v_ν and v_{ν^*} to be real and non-negative, i.e.

$$v_\nu \overset{!}{\in}]0, \infty[, \tag{3.52}$$

without loss of generality. Then, due to Equation (3.48), one also has $v'_\nu \in \mathbb{R}$. More specifically, due to the positivity of v_ν and (3.46), the sign of v'_{ν^*} is given by

$$\operatorname{sgn}(v'_{\nu^*}) = -\operatorname{sgn}\left(2 + |M| \frac{e_\nu - \mu}{g N_0}\right). \tag{3.53}$$

The real equivalents of the previous conditions then read

$$-2\left(2 + |M| \frac{e_\nu - \mu}{g N_0}\right) = \frac{v'_{\nu^*}}{v_\nu} + \frac{v_\nu}{v'_{\nu^*}} \tag{3.54}$$

$$v_\nu = v_{\nu^*} \quad \wedge \quad v'_\nu = v'_{\nu^*} \tag{3.55}$$

$$v_\nu^2 - v_{\nu^*}'^2 = 1. \tag{3.56}$$

With the help of (3.56), Equation (3.54) is expressed as a polynomial of degree two in v_ν^2, solving which yields

$$v_\nu^2 = \frac{1}{2} \pm \frac{1}{2} \sqrt{1 + \frac{1}{\left(2 + |M| \frac{e_\nu - \mu}{g N_0}\right)^2 - 1}}, \tag{3.57}$$

where the solution with the minus sign is discarded as v_ν^2 is positive. With the symmetry (3.55) and the sign convention (3.52), the Bogoliubov coefficients finally evaluate to

$$\left.\begin{matrix} v_\nu \\ -\operatorname{sgn}\left(2 + |M| \frac{e_\nu - \mu}{g N_0}\right) v'_\nu \end{matrix}\right\} = \sqrt{\pm \frac{1}{2} + \frac{1}{2} \sqrt{1 + \frac{1}{\left(2 + |M| \frac{e_\nu - \mu}{g N_0}\right)^2 - 1}}}. \tag{3.58}$$

The results for the Bogoliubov operators $\hat{B}_\nu$ and coefficients v_ν,v'_ν are now inserted into the thermal energy operator (3.41). Since the coefficients of the off-diagonal operator pairs vanish due to (3.42) and by using the bosonic commutation relations (3.39), one gets

$$\begin{aligned} \hat{T} \approx & N_0 \left(\frac{g N_0}{2|M|} + e_0 - \mu\right) + \sum_{\nu \neq 0} \left(|v'_{\nu^*}|^2 \left(\frac{2 g N_0}{|M|} + e_\nu - \mu\right) + \left(v_\nu v'_{\nu^*} + v_\nu^* v_{\nu^*}'^*\right) \frac{g N_0}{2|M|} \right) \\ & + \sum_{\nu \neq 0} \hat{B}_\nu^\dagger \hat{B}_\nu \left(\left(|v_\nu|^2 + |v'_{\nu^*}|^2\right) \left(\frac{2 g N_0}{|M|} + e_\nu - \mu\right) + \left(v'_\nu v_{\nu^*} + v_\nu'^* v_{\nu^*}^* + v_\nu v'_{\nu^*} + v_\nu^* v_{\nu^*}'^*\right) \frac{g N_0}{2|M|} \right). \end{aligned} \tag{3.59}$$

With the realness (3.52) and symmetry (3.55) of the Bogoliubov coefficients this expression further simplifies to

$$\hat{T} \approx N_0 \left(\frac{gN_0}{2|M|} + e_0 - \mu \right) + \sum_{\nu \neq 0} \left(v_\nu'^2 \left(\frac{2gN_0}{|M|} + e_\nu - \mu \right) + v_\nu v_\nu' \frac{gN_0}{|M|} \right)$$
$$+ \sum_{\nu \neq 0} \hat{B}_\nu^\dagger \hat{B}_\nu \left(\left(v_\nu^2 + v_\nu'^2 \right) \left(\frac{2gN_0}{|M|} + e_\nu - \mu \right) + v_\nu' v_\nu \frac{2gN_0}{|M|} \right). \tag{3.60}$$

Lastly, inserting the explicit expressions (3.58) for the Bogoliubov coefficients therein and performing some algebraic rearrangements finally yields the form

$$\hat{T} \approx N_0 \left(\frac{gN_0}{2|M|} + e_0 - \mu \right) + \sum_{\nu \neq 0} \operatorname{sgn} \left(2 + |M| \frac{e_\nu - \mu}{gN_0} \right) \left(\frac{\varepsilon_\nu - \sqrt{\varepsilon_\nu^2 + \left(\frac{gN_0}{|M|} \right)^2}}{2} + \varepsilon_\nu \hat{B}_\nu^\dagger \hat{B}_\nu \right), \tag{3.61}$$

which is quadratic and diagonal in the bosonic ladder operators $\hat{B}_\nu$. Here, the Bogoliubov dispersion

$$\varepsilon_\nu \equiv \sqrt{\left(2\frac{gN_0}{|M|} + e_\nu - \mu \right)^2 - \left(\frac{gN_0}{|M|} \right)^2} \tag{3.62}$$

is introduced.

3.1.2 Grand-canonical potential and ground state occupation

The approximate expression (3.61) for the thermal energy operator is identified with the form (3.1) via the relabeling

$$\hat{B}_\nu \to \hat{b}_\nu \tag{3.63}$$

$$N_0 \left(\frac{gN_0}{2|M|} + e_0 - \mu \right) + \sum_{\nu \neq 0} \operatorname{sgn} \left(2 + |M| \frac{e_\nu - \mu}{gN_0} \right) \frac{\varepsilon_\nu - \sqrt{\varepsilon_\nu^2 + \left(\frac{gN_0}{|M|} \right)^2}}{2} \to \varepsilon \tag{3.64}$$

$$\operatorname{sgn} \left(2 + |M| \frac{e_\nu - \mu}{gN_0} \right) \varepsilon_\nu \to \varepsilon_\nu. \tag{3.65}$$

As the energies ε_ν need to be positive for the geometric series to converge in the partition function (3.2), one reads out, that the sign $2 + |M| \frac{e_\nu - \mu}{gN_0}$ needs to be positive for all $\nu \neq 0$. Equivalently, the variational parameter N_0 has to fulfill the condition

$$N_0 > \frac{|M|(\mu - e_1)}{2g}, \tag{3.66}$$

where $e_1 = \min_{\nu \neq 0}$ is set to be the next smallest energy after e_0. Consequently, one gets for the grand-canonical potential (3.3) the approximate identity

$$\Omega \approx N_0 \left(\frac{gN_0}{2|M|} + e_0 - \mu \right) + \sum_{\nu \neq 0} \frac{\varepsilon_\nu - \sqrt{\varepsilon_\nu^2 + \left(\frac{gN_0}{|M|} \right)^2}}{2} + k_B T \sum_{\nu \neq 0} \ln \left(1 - e^{-\frac{\varepsilon_\nu}{k_B T}} \right). \tag{3.67}$$

Its three additive components are labeled the mean-field contribution, quantum fluctuations and thermal fluctuations, from left to right.

The approximations (3.16), (3.23), (3.25) and (3.27), which were made to enable the evaluation of the trace in the partition function, selfevidently cause a deviation from the exact solution for the grand-canonical potential. The variational parameter N_0 constitutes a degree of freedom, which is now chosen such as to minimize the compound effect of those approximations. Mathematically, this amounts to finding the global minimum of the difference of the actual and the approximated grand-canonical potential with respect to N_0. Here, it is assumed, that the local extremum (or saddle point), that one gets by extremizing (3.67) like

$$0 \stackrel{!}{=} \frac{d\Omega}{dN_0}, \tag{3.68}$$

is the global minimum. An approximation scheme is employed to perform this extremizition, based on the assumption, that the mean-field contribution of the grand-canonical potential is larger than the fluctuations. This assumption is integrated into the formalism by introducing an artificial smallness parameter $\eta \in \mathbb{R}$ and defining the effective grand-canonical potential

$$\Omega_{\text{eff}}(\eta, N_0) \equiv N_0 \left(\frac{gN_0}{2|M|} + e_0 - \mu \right) + \eta \sum_{\nu \neq 0} \left(\frac{\varepsilon_\nu - \sqrt{\varepsilon_\nu^2 + \left(\frac{gN_0}{|M|}\right)^2}}{2} + k_B T \ln\left(1 - e^{-\frac{\varepsilon_\nu}{k_B T}}\right) \right). \tag{3.69}$$

(The functional dependence of the effective grand-canonical potential on any other thermodynamical variables is omitted in the notation for clarity.) It is related to the actual grand-canonical potential throuh Equation (3.67) as

$$\Omega \approx \Omega_{\text{eff}}|_{\eta=1}\,. \tag{3.70}$$

Therewith, the comparative smallness of the fluctuations is expressed as

$$\frac{\Omega_{\text{eff}}(0, N_0)}{\Omega_{\text{eff}}(1, N_0)} \stackrel{!}{\approx} 1. \tag{3.71}$$

The extremization (3.68) then amounts to finding the implicit function $N_0(\eta)$ which fulfills

$$0 = \frac{d\Omega_{\text{eff}}}{dN_0}(\eta, N_0(\eta)) \tag{3.72}$$

and evaluating it at $\eta = 1$. Due to the assumed smallness of the fluctuations (3.71), this implicit function is evaluated only up to first order in the smallness parameter

$$N_0(\eta) \approx N_0(0) + \eta \frac{dN_0}{d\eta}(0). \tag{3.73}$$

The two parameters $N_0(0)$ and $\frac{dN_0}{d\eta}(0)$ are determined in the following. The derivative of the effective grand-canonical potential (3.69) with respect to the variational parameter N_0 reads

$$\frac{d\Omega_{\text{eff}}}{dN_0}(\eta, N_0) = \frac{gN_0}{|M|} + e_0 - \mu + \eta \sum_{\nu \neq 0} \left(\frac{d\varepsilon_\nu}{dN_0} \left(\frac{1}{2} + \frac{1}{e^{\frac{\varepsilon_\nu}{k_B T}} - 1} \right) - \frac{g}{|M|} \right), \tag{3.74}$$

with the derivative

$$\frac{d\varepsilon_\nu}{dN_0} = \frac{1}{\varepsilon_\nu} \frac{g}{|M|} \left(3\frac{gN_0}{|M|} + 2(e_\nu - \mu) \right) \tag{3.75}$$

of the Bogoliubov energies (3.62). Evaluating (3.74) at $\eta = 0$ and solving for $N_0(0)$ yields

$$N_0(0) = \frac{|M|}{g}(\mu - e_0). \tag{3.76}$$

From the definition (3.72) of the implicit function $N_0(\eta)$ follows the differentiation rule

$$\frac{dN_0}{d\eta}(\eta) = -\frac{\frac{d^2\Omega}{dN_0 d\eta}}{\frac{d^2\Omega}{dN_0^2}}(\eta, N_0(\eta)). \tag{3.77}$$

The derivative of (3.74) with respect to N_0 evaluated at $\eta = 0$ and $N_0 = N(0)$ from (3.76) simply reads

$$\frac{d^2\Omega}{dN_0^2}(0, N_0(0)) = \frac{g}{|M|}. \tag{3.78}$$

Using the expression (3.76) for $N(0)$, two auxiliary results regarding the Bogoliubov dispersion (3.62) are derived:

$$\varepsilon_\nu|_{N_0=N_0(0)} = \sqrt{(e_\nu - e_0)((e_\nu - e_0) + 2(\mu - e_0))} \tag{3.79}$$

$$\left.\frac{d\varepsilon_\nu}{dN_0}\right|_{N_0=N_0(0)} = \frac{1}{\varepsilon_\nu|_{N_0=N_0(0)}} \frac{g}{|M|} \left((\mu - e_0) + 2(e_\nu - e_0)\right). \tag{3.80}$$

With their help, the derivative of (3.74) with respect to η evaluated at $\eta = 0$ and $N_0 = N(0)$ from (3.76) yields

$$\frac{d^2\Omega}{dN_0 d\eta}(0, N_0(0)) = \frac{g}{|M|} \sum_{\nu \neq 0} \left(\frac{(\mu - e_0) + 2(e_\nu - e_0)}{\varepsilon_\nu|_{N_0=N_0(0)}} \left(\frac{1}{2} + \frac{1}{e^{\frac{\varepsilon_\nu|_{N_0=N_0(0)}}{k_B T}} - 1} \right) - 1 \right). \tag{3.81}$$

Inserting the double deriavtives (3.78) and (3.81) of the effectice grand-canonical potential back into Equation (3.77) gives the second parameter

$$\frac{dN_0}{d\eta}(0) = \sum_{\nu \neq 0} \left(1 - \frac{(\mu - e_0) + 2(e_\nu - e_0)}{\varepsilon_\nu|_{N_0=N_0(0)}} \left(\frac{1}{2} + \frac{1}{e^{\frac{\varepsilon_\nu|_{N_0=N_0(0)}}{k_B T}} - 1} \right) \right). \tag{3.82}$$

The respective expressions (3.76) and (3.82) for the parameters $N_0(0)$ and $\frac{dN_0}{d\eta}(0)$ are inserted back into the approximate expression (3.73) for the implicit function $N_0(\eta)$. Evaluation at $\eta = 1$ then finally gives the approximation

$$N_0 \approx \frac{|M|}{g}(\mu - e_0) + \sum_{\nu \neq 0} \left(1 - \frac{(\mu - e_0) + 2(e_\nu - e_0)}{\sqrt{(e_\nu - e_0)((e_\nu - e_0) + 2(\mu - e_0))}} \left(\frac{1}{2} + \frac{1}{e^{\frac{\sqrt{(e_\nu - e_0)((e_\nu - e_0) + 2(\mu - e_0))}}{k_B T}} - 1} \right) \right) \tag{3.83}$$

for the value of the variational parameter N_0, that extremizes the effective grand-canonical potential (3.67). It remains to evaluate the grand-canonical potential (3.67) at the newly found extremizing variational parameter (3.83). This is done in an approximate manner due to the smallness (3.71) of the fluctuations. The implicit function $N_0(\eta)$ up to first order in η (3.73) is inserted into the effective grand-canonical potential (3.69) and sorted by orders of the artificial smallness parameter η:

$$
\begin{aligned}
\Omega_{\text{eff}}(\eta, N_0(\eta)) \approx & \Omega_{\text{eff}}\left(\eta, N_0(0) + \eta\frac{dN_0}{d\eta}(0)\right) \\
= & \left(N_0(0) + \eta\frac{dN_0}{d\eta}(0)\right)\left(\frac{g}{2|M|}\left(N_0(0) + \eta\frac{dN_0}{d\eta}(0)\right) + e_0 - \mu\right) \\
& + \eta\sum_{\nu\neq 0}\left(\frac{\varepsilon_\nu - \sqrt{\varepsilon_\nu^2 + \left(\frac{gN_0}{|M|}\right)^2}}{2} + k_BT\ln\left(1 - e^{-\frac{\varepsilon_\nu}{k_BT}}\right)\right)\Bigg|_{N_0 = N_0(0) + \eta\frac{dN_0}{d\eta}(0)} \\
= & N_0(0)\left(\frac{g}{2|M|}N_0(0) + e_0 - \mu\right) + \eta\frac{dN_0}{d\eta}(0)\left(\frac{g}{|M|}N_0(0) + e_0 - \mu\right) \\
& + \eta\sum_{\nu\neq 0}\left(\frac{\varepsilon_\nu - \sqrt{\varepsilon_\nu^2 + \left(\frac{gN_0}{|M|}\right)^2}}{2} + k_BT\ln\left(1 - e^{-\frac{\varepsilon_\nu}{k_BT}}\right)\right)\Bigg|_{N_0 = N_0(0)} + \mathcal{O}(\eta^2)
\end{aligned} \tag{3.84}
$$

Finally, by evaluating this identity at $\eta = 1$ with the help of the respective expressions (3.76) and (3.82) for the parameters $N_0(0)$ and $\frac{dN_0}{d\eta}(0)$, one gets the approximate expression

$$
\begin{aligned}
\Omega \approx \Omega_{\text{eff}}(1, N_0(1)) \approx & -\frac{|M|}{2g}(\mu - e_0)^2 \\
& + \sum_{\nu\neq 0}\frac{\sqrt{(e_\nu - e_0)((e_\nu - e_0) + 2(\mu - e_0))} - (\mu - e_0) - (e_\nu - e_0)}{2} \\
& + k_BT\sum_{\nu\neq 0}\ln\left(1 - e^{-\frac{\sqrt{(e_\nu - e_0)((e_\nu - e_0) + 2(\mu - e_0))}}{k_BT}}\right)
\end{aligned} \tag{3.85}
$$

for the grand-canonical potential, due to Equation (3.70).

3.2 Super-canonical description in a box

Now, analogous to the preceding derivation of the grand-canonical potential of a gas on an arbitrary manifold, the super-canonical potential is evaluated in the specific case of an n-dimensional box with periodic boundary conditions. To be precise, "box" means, that the spatial domain of the function of ladder operators $\hat{a}_\bullet$ in the second quantized description and consequently of the first quantized wavefunctions φ is set to $M = [0, L]^n$ with $L \in [0, \infty[$. The "periodic" boundary conditions are specified as

$$
\hat{a}_\bullet|_{x_i = 0} = \hat{a}_\bullet|_{x_i = L} \tag{3.86}
$$

for all $i \in \{1 \cdots n\}$, which then also applies to the first quantized wavefunction φ.

For the box, the Laplace-Beltrami differential operator on M is a simple Laplace operator. A complete set of solutions to its eigenvalue problem (3.4), which comply with the periodic boundary conditions, is then given by plane waves

$$
\psi_k(x) \equiv L^{-\frac{n}{2}}e^{ik\cdot x} \tag{3.87}
$$

and energies

$$
e_k = \frac{\hbar^2\|k\|^2}{2m} \tag{3.88}
$$

with $k \in \frac{2\pi}{L}\mathbb{Z}^n$. These plane waves are orthonormal with respect to the scalar product (3.6). They also have the property

$$
\psi_k^* = \psi_{-k}, \tag{3.89}
$$

meaning that (3.8) is fulfilled with $k^* = -k$. Additionally, they are also eigenfunctions of the gradient:

$$
\nabla\psi_k = ik\psi_k. \tag{3.90}
$$

3.2.1 Super-canonical potential and ground state occupation

As a consequence, the procedure for simplifying the thermal energy operator, which was undergone in the case of a grandcanonical description on an arbitrary manifold, may be emulated to a great extent. Starting out by specializing on $M = [0, L]^n$ in the generic expression (2.5) for the super canonical potential, one has

$$\hat{T} = \int\limits_{[0,L]^n} \hat{a}_x^\dagger \left(-\frac{\hbar^2}{2m}\Delta - i\hbar u \cdot \nabla - \mu \right) \hat{a}_x \, dx + \frac{1}{2} \int\limits_{[0,L]^n} \int\limits_{[0,L]^n} \hat{a}_x^\dagger \hat{a}_{x'}^\dagger V(x - x') \hat{a}_x \hat{a}_{x'} \, dx \, dx'. \tag{3.91}$$

Analogous to (3.10), the spatial dependence of $\hat{a}_\bullet$ is expanded with the help of the specific eigenfunctions (3.88). Due to (3.90), the contribution of u to $\hat{T}$ simplifies just like the kinetic contribution, leading to the thermal energy operator

$$\hat{T} = \sum_\kappa \hat{b}_\kappa^\dagger \hat{b}_\kappa (e_\kappa + \hbar u \cdot \kappa - \mu) + \frac{1}{2} \sum_{\nu,\nu',\kappa,\kappa'} \hat{b}_\nu^\dagger \hat{b}_{\nu'}^\dagger \hat{b}_\kappa \hat{b}_{\kappa'} \int\limits_{[0,L]^n} \int\limits_{[0,L]^n} \psi_\nu^*(x) \psi_{\nu'}^*(x) V(x - x') \psi_\kappa(x) \psi_{\kappa'}(x) \, dx \, dx', \tag{3.92}$$

where each of the summations over κ, κ', ν or ν' now runs over the set $\frac{2\pi}{L}\mathbb{Z}^n$. Now, the approximations (3.16), (3.23), (3.25) are applied completely analogously to the grandcanonical description on an arbitrary manifold. Notably, equation (3.27) does not constitute an approximation, as for the box ψ_0 is a constant. In total, as an analogon to Equation (3.32), one gets the expression

$$\hat{T} \approx N_0 \left(\frac{gN_0}{2L^n} - \mu \right) + \sum_{k \neq 0} \left(\hat{b}_k^\dagger \hat{b}_k \left(\frac{2gN_0}{L^n} + e_k + \hbar u \cdot k - \mu \right) + \frac{gN_0}{2L^n} \left(\hat{b}_k^\dagger \hat{b}_{-k}^\dagger + \hat{b}_k \hat{b}_{-k} \right) \right). \tag{3.93}$$

Now the Bogoliubov transformation (3.33) is performed with the same coefficients as in (3.58). The expression (3.93) differs from (3.32) by the additional term $\hbar u \cdot \sum\limits_{k \neq 0} k \hat{b}_k^\dagger \hat{b}_k$, which might lead to complications with the Bogoliubov transformation. Inserting the Bogoliubov transformation into the additional term, the auxiliary calculation

$$\begin{aligned}
\sum_{k \neq 0} k \hat{b}_k^\dagger \hat{b}_k &= \sum_{k \neq 0} k \left(v_k^2 \hat{B}_k^\dagger \hat{B}_k + v_k'^2 \hat{B}_{-k} \hat{B}_{-k}^\dagger + v_k v_k' \left(\hat{B}_k^\dagger \hat{B}_{-k}^\dagger + \hat{B}_k \hat{B}_{-k} \right) \right) \\
&= \sum_{k \neq 0} k \left(v_k^2 \hat{B}_k^\dagger \hat{B}_k - v_k'^2 \hat{B}_k \hat{B}_k^\dagger + \frac{v_k v_k'}{2} \left(\left[\hat{B}_k^\dagger, \hat{B}_{-k}^\dagger \right] + \left[\hat{B}_k \hat{B}_{-k} \right] \right) \right) \\
&= \sum_{k \neq 0} (v_k^2 - v_k'^2) k \hat{B}_k^\dagger \hat{B}_k + k v_k^2 \\
&= \sum_{k \neq 0} k \hat{B}_k^\dagger \hat{B}_k
\end{aligned} \tag{3.94}$$

is performed, where the symmetry $\sum\limits_{k \neq 0} k \cdots = - \sum\limits_{-k \neq 0} k \cdots$ was used in the second equality. Therewith it becomes evident, that the former choice for the coefficients v_k and v_k' still diagonalizes the thermal energy operator, leading to the expression

$$\hat{T} \approx N_0 \left(\frac{gN_0}{2L^n} - \mu \right) + \sum_{k \neq 0} \frac{\varepsilon_k - \sqrt{\varepsilon_k^2 + \left(\frac{gN_0}{L^n} \right)^2}}{2} + \sum_{k \neq 0} \left(\varepsilon_k + \hbar u \cdot k \right) \hat{B}_k^\dagger \hat{B}_k, \tag{3.95}$$

which is the analogon to (3.61), where the Bogoliubov dispersion ε_k remains unaltered as in (3.62). The thermal energy operator is now approximately of the desired shape (3.1) and the effective super-canonical potential evaluates to

$$\Omega \approx N_0 \left(\frac{gN_0}{2L^n} - \mu \right) + \sum_{k \neq 0} \frac{\varepsilon_k - \sqrt{\varepsilon_\nu^2 + \left(\frac{gN_0}{L^n} \right)^2}}{2} + k_B T \sum_{k \neq 0} \ln \left(1 - e^{-\frac{\varepsilon_k + \hbar u \cdot k}{k_B T}} \right). \tag{3.96}$$

This expression only differs from its analogon (3.67) in the grand-canonical description on an arbitrary manifold in that the thermal fluctuations contain $\varepsilon_k + \hbar u \cdot k$ instead of only ε_ν. This difference only marginally affects the evaluation of the variational parameter N_0, leading to the result

$$N_0 \approx \frac{L^n \mu}{g} + \sum_{k \neq 0} \left(1 - \frac{\mu + 2e_k}{\sqrt{e_k(e_k + 2\mu)}} \left(\frac{1}{2} + \frac{1}{e^{\frac{\sqrt{e_k(e_k+2\mu)} + \hbar u \cdot k}{k_B T}} - 1} \right) \right), \tag{3.97}$$

as the analogon to (3.83). Lastly, inserting the optimized choice for the variational parameter into the effective super-canonical potential (3.96) approximately yields

$$\Omega \approx -\frac{L^n \mu^2}{2g} + \sum_{k \neq 0} \frac{\sqrt{e_k(e_k + 2\mu)} - \mu - e_k}{2} + k_B T \sum_{k \neq 0} \ln \left(1 - e^{-\frac{\sqrt{e_k(e_k+2\mu)} + \hbar u \cdot k}{k_B T}} \right). \tag{3.98}$$

This expression for the super-canonical potential is the analogon to (3.85). Both the ground state occupation and the super-canonical potential decompose additively into three contributions: The mean-field term, that doesn't depend on the quantum numbers; the thermal fluctuations, which vanish at $T = 0$; and the remaining term, called quantum fluctuations.

3.2.2 Removing divergencies

In both of the expressions (3.97) for the varitional parameter N_0 and (3.98) for the super-canonical potential of an n-dimensional box, the mean-field term and the quantum fluctuations are anticipated to be divergent. Cutoff regularization is employed to quantitatively describe said divergencies and to remove them in retrospect.

Interaction strength The origin of the divergencies lies in Equation (3.25), where the general interaction potential V is approximated by contact interaction. So far, for this approximation, it was only advertised, that the interaction strength g ought to be chosen, such that the low-energy limit $a_s(0)$ of the scattering length of V is preserved. It remains to derive the consequent functional dependence of g on $a_s(0)$.

The scattering theory, in two and three dimensions, with a general two-particle interaction potential is treated in detail in Appendix D, which is now specialized on contact iteraction. For a given wavenumber κ, equation (D.32) relates the s-wave scattering length $a_s(\kappa)$ to the scattering total cross section $\sigma(\kappa)$, which is in turn related to the scattering amplitude f via equation (D.42). An expression for f is given by equation (D.38). Inserting contact interaction into (D.38) yields

$$f = C_n g \phi(0), \tag{3.99}$$

showing that the scattering amplitude becomes a constant function of the directions $\partial B_1(0)$. Consequently, equations (D.32) and (D.42) simplify to

$$|a_s(\kappa)| \approx |f|. \tag{3.100}$$

The value of the wavefunction ϕ at the origin is determined by inserting contact interaction into (D.22) and evaluating the Lippmann-Schwinger equation (D.21) at $x = 0$. Solving for $\phi(0)$ then yields

$$\phi(0) = \frac{1}{1 - \frac{m}{\hbar^2} g G_\kappa(0)} \tag{3.101}$$

To evaluate $G_\kappa(0)$, the expression (D.5) for the Green's function of the Laplace operator is used. Therein, at equal arguments $x = x' = 0$, the integrand only depends on $\|q\|$, such that the angular integral is factored out after substituting spherical coordinates, yielding

$$
\begin{aligned}
G_\kappa(0) &= (2\pi)^{-n} \int\limits_{\mathbb{R}^n} \frac{1}{\kappa^2 - \|q\|^2}\, dq \\
&= (2\pi)^{-n} |\partial B_1(0)| \lim_{\Lambda\to\infty} \int\limits_0^\Lambda \frac{q^{n-1}}{\kappa^2 - q^2}\, dq \\
&= -\frac{1}{2\pi} \lim_{\Lambda\to\infty} \begin{cases} \frac{\Lambda}{\pi} & n = 3 \\ \ln\left(\frac{\Lambda}{\kappa}\right) & n = 2 \end{cases}.
\end{aligned} \tag{3.102}
$$

In the last equality, the auxiliary calculations

$$
\int\limits_0^\Lambda \frac{q}{\kappa^2 - q^2}\, dq = \int\limits_0^{\frac{\Lambda}{\kappa}} \frac{x}{1 - x^2}\, dq = -\frac{1}{2} \ln\left(\left|1 - \left(\frac{\Lambda}{\kappa}\right)^2\right|\right) \tag{3.103}
$$

for two dimensions and

$$
\begin{aligned}
\int\limits_0^\Lambda \frac{q^2}{\kappa^2 - q^2}\, dq &= \kappa \int\limits_0^{\frac{\Lambda}{\kappa}} \underbrace{\frac{x^2}{1 - x^2}}_{=-1+\frac{1}{2}\frac{1}{x+1}-\frac{1}{2}\frac{1}{x-1}} dx \\
&= \kappa \left[-x + \frac{1}{2}\ln(|x+1|) - \frac{1}{2}\ln(|x-1|)\right]_0^{\frac{\Lambda}{\kappa}} \\
&= -\Lambda + \frac{\kappa}{2} \ln\left(\left|\frac{\kappa + \Lambda}{\kappa - \Lambda}\right|\right)
\end{aligned} \tag{3.104}
$$

for three dimensions were used. Consecutively inserting Equations (3.99), (3.101) and (3.102) into (3.100) leads to the expression

$$
\begin{aligned}
\frac{1}{g} &= \left|\frac{C_n}{a_s(\kappa)}\right| + \frac{m}{\hbar^2} G_\kappa(0) \\
&= \frac{m}{2\pi\hbar^2} \begin{cases} \frac{1}{2|a_s(\kappa)|} + \frac{\kappa}{2\pi} \lim\limits_{\Lambda\to\infty} \ln\left(\left|\frac{\kappa+\Lambda}{\kappa-\Lambda}\right|\right) - \frac{1}{\pi} \lim\limits_{\Lambda\to\infty} \Lambda & n = 3 \\ \frac{\sqrt{\pi}}{\sqrt{\kappa}|a_s(\kappa)|} + \ln(\kappa) - \lim\limits_{\Lambda\to\infty} \ln(\Lambda) & n = 2 \end{cases} \\
&\underset{\kappa\to 0}{\to} \frac{m}{2\pi\hbar^2} \begin{cases} \frac{1}{2|a_s(0)|} - \frac{1}{\pi} \lim\limits_{\Lambda\to\infty} \Lambda & n = 3 \\ -\ln\left(\frac{a_s(0)}{2}\right) - \gamma - \lim\limits_{\Lambda\to\infty} \ln(\Lambda) & n = 2 \end{cases}
\end{aligned} \tag{3.105}
$$

for the inverse interaction strength. While the low energy limit $\kappa \to 0$ is trivially performed in three dimensions, the limit in two dimensions is found by comparison with [15, eq. 43]. This confirms the divergence of the mean-field contributions of the ground state occupation and of the super-canonical potential.

Quantum fluctuations The quantum fluctuations in (3.97) and (3.98) are evaluated approximately. To this end, the summation over the grid $\frac{2\pi}{L}\mathbb{Z}^n$ is construed as a Riemann sum approximating the integration with respect to k over $\mathbb{R}^n$. As the integrands then only depend on the absolute value $\|k\|$ through e_k, the angular integral is factored out after switching to spherical coordniates. In total one gets the approximation

$$
\sum_{k\in\frac{2\pi}{L}\mathbb{Z}^n\setminus\{0\}} \cdots(\|k\|) \approx \left(\frac{L}{2\pi}\right)^n \int\limits_{\mathbb{R}^n} dk\ \cdots(\|k\|) = \left(\frac{L}{2\pi}\right)^n |\partial B_1(0)| \lim_{\Lambda\to\infty} \int\limits_0^\Lambda dk\ \cdots(k) k^{n-1}, \tag{3.106}
$$

with $|\partial_1 B(0)|$ denoting the surface area of an n-dimensional unit sphere, e.g. $|\partial_1 B(0)| = 2\pi$ for $n = 2$ and $|\partial_1 B(0)| = 4\pi$ for $n = 3$. Using the approximation (3.106) of the summation and explicitly writing out the energies e_k from (3.88) in the quantum fluctions of the super-canonical potential (3.98) yields

$$\sum_{k\neq 0} \frac{\sqrt{e_k(e_k+2\mu)}-\mu-e_k}{2} \approx \left(\frac{L}{2\pi}\right)^n |\partial B_1(0)| \int_0^\Lambda k^{n-1} \frac{\sqrt{\frac{\hbar^2k^2}{2m}\left(\frac{\hbar^2k^2}{2m}+2\mu\right)}-\mu-\frac{\hbar^2k^2}{2m}}{2}\, dk. \tag{3.107}$$

Analogously, for the quantum fluctuations of the ground-state occupation (3.97), one gets

$$\sum_{k\neq 0}\left(1-\frac{e_k+\frac{\mu}{2}}{\sqrt{e_k(e_k+2\mu)}}\right) \approx \left(\frac{L}{2\pi}\right)^n |\partial B_1(0)| \int_0^\Lambda k^{n-1}\left(1-\frac{\frac{\hbar^2k^2}{2m}+\frac{\mu}{2}}{\sqrt{\frac{\hbar^2k^2}{2m}\left(\frac{\hbar^2k^2}{2m}+2\mu\right)}}\right). \tag{3.108}$$

Equations (3.107) and (3.108) are evaluated in the following for $n \in \{2, 3\}$.

n=3 : The quantum fluctuations of the super-canonical potential are investigated in three dimensions. First, the auxiliary calculation

$$\begin{aligned}
&\int_0^{\frac{\hbar^2\Lambda^2}{4m\mu}} x\sqrt{1+x}\, dx \;=\; \int_1^{\frac{\hbar^2\Lambda^2}{4m\mu}+1} (x-1)\sqrt{x}\, dx \;=\; \left[\frac{2}{5}x^{\frac{5}{2}}-\frac{2}{3}x^{\frac{3}{2}}\right]_1^{\frac{\hbar^2\Lambda^2}{4m\mu}+1} \\
=\; &\underbrace{\sqrt{1+\frac{4m\mu}{\hbar^2\Lambda^2}}}_{=1+\frac{1}{2}\left(\frac{\hbar\Lambda}{\sqrt{4m\mu}}\right)^{-2}-\frac{1}{8}\left(\frac{\hbar\Lambda}{\sqrt{4m\mu}}\right)^{-4}+\mathcal{O}(\Lambda^{-6})} \left(\frac{2}{5}\left(\frac{\hbar\Lambda}{\sqrt{4m\mu}}\right)^5+\frac{2}{15}\left(\frac{\hbar\Lambda}{\sqrt{4m\mu}}\right)^3-\frac{4}{15}\frac{\hbar\Lambda}{\sqrt{4m\mu}}\right)+\frac{4}{15} \\
=\; &\frac{2}{5}\left(\frac{\hbar\Lambda}{\sqrt{4m\mu}}\right)^5+\frac{1}{3}\left(\frac{\hbar\Lambda}{\sqrt{4m\mu}}\right)^3-\frac{1}{4}\frac{\hbar\Lambda}{\sqrt{4m\mu}}+\frac{4}{15}+\mathcal{O}\left(\Lambda^{-1}\right)
\end{aligned}$$

is performed, which is in turn used in the second auxiliary calculation

$$\begin{aligned}
&\int_0^\Lambda k^2 \frac{\hbar k}{\sqrt{2m}}\sqrt{\frac{\hbar^2k^2}{2m}+2\mu}\, dk \\
=&\mu\left(\frac{\hbar}{\sqrt{4m\mu}}\right)^{-3}\int_0^{\frac{\hbar^2\Lambda^2}{4m\mu}} x\sqrt{1+x}\, dx \\
=&\frac{1}{5}\frac{\hbar^2}{2m}\Lambda^5+\frac{1}{3}\mu\Lambda^3-\frac{1}{2}\mu^2\frac{2m}{\hbar^2}\Lambda+\frac{4}{15}\mu\left(\frac{\hbar}{\sqrt{4m\mu}}\right)^{-3}+\mathcal{O}\left(\Lambda^{-1}\right),
\end{aligned}$$

where only basic algebra and integration methods were used. Then, inserting $n = 3$ and the auxiliary result into (3.107) yields

$$
\begin{aligned}
&\sum_{k\neq 0}\frac{\sqrt{e_k(e_k+2\mu)}-\mu-e_k}{2}\\
\approx&\frac{L^3}{(2\pi)^2}\lim_{\Lambda\to\infty}\left(\frac{1}{5}\frac{\hbar^2}{2m}\Lambda^5+\frac{1}{3}\mu\Lambda^3-\frac{1}{2}\mu^2\frac{2m}{\hbar^2}\Lambda+\frac{4}{15}\mu\left(\frac{\hbar}{\sqrt{4m\mu}}\right)^{-3}+\left[\frac{\hbar^2}{2m}\frac{1}{5}k^5+\mu\frac{1}{3}k^3\right]_0^{\Lambda}\right)\\
=&\frac{L^3\mu}{15\pi^2}\left(\frac{\hbar}{\sqrt{4m\mu}}\right)^{-3}-\frac{L^3\mu^2}{8\pi^2}\frac{2m}{\hbar^2}\lim_{\Lambda\to\infty}\Lambda\\
=&\frac{mL^3\mu^2}{4\pi^2\hbar^2}\left(\frac{32}{15}\frac{\sqrt{m\mu}}{\hbar}-\lim_{\Lambda\to\infty}\Lambda\right),
\end{aligned}
\tag{3.109}
$$

thereby revealing the divergent nature of the quantum fluctuations of Ω.

The quantum fluctuations of N_0 are treated analogously. With the auxiliary calculation

$$
\begin{aligned}
&\int_0^{\Lambda}k^2\frac{k^2+\frac{m\mu}{\hbar^2}}{\sqrt{k^2(k^2+4\frac{m\mu}{\hbar^2})}}\,dk\\
=&\int_0^{\Lambda}\left(k^2+\frac{m\mu}{\hbar^2}\right)\frac{d}{dk}\sqrt{k^2+4\frac{m\mu}{\hbar^2}}\,dk\\
=&\left[\left(k^2+\frac{m\mu}{\hbar^2}\right)\sqrt{k^2+4\frac{m\mu}{\hbar^2}}\right]_0^{\Lambda}-\frac{2}{3}\int_0^{\Lambda}\frac{d}{dk}\left(k^2+4\frac{m\mu}{\hbar^2}\right)^{\frac{3}{2}}\,dk\\
=&\underbrace{\sqrt{1+4\frac{m\mu}{\hbar^2\Lambda^2}}}_{=1+2\frac{m\mu}{\hbar^2\Lambda^2}+\mathcal{O}(\Lambda^{-4})}\frac{\Lambda^3-5\frac{m\mu}{\hbar^2}\Lambda}{3}+\frac{10}{3}\left(\frac{\sqrt{m\mu}}{\hbar}\right)^3\\
=&\frac{\Lambda^3}{3}-\frac{m\mu}{\hbar^2}\Lambda+\frac{10}{3}\left(\frac{\sqrt{m\mu}}{\hbar}\right)^3+\mathcal{O}\left(\Lambda^{-1}\right)
\end{aligned}
$$

and by inserting $n=3$ into the quantum fluctuations (3.108), one gets

$$
\sum_{k\neq 0}\left(1-\frac{e_k+\frac{\mu}{2}}{\sqrt{e_k(e_k+2\mu)}}\right)=\frac{L^3}{2\pi^2}\left(\frac{m\mu}{\hbar^2}\lim_{\Lambda\to\infty}\Lambda-\frac{10}{3}\left(\frac{\sqrt{m\mu}}{\hbar}\right)^3\right).
\tag{3.110}
$$

n=2 : The quantum fluctuations of the two-dimensional box are evaluated analogous to the three-dimenional case. For the super-canonical potential, the auxiliary calculation

$$
\begin{aligned}
&\int_0^{\frac{\hbar\Lambda}{\sqrt{4m\mu}}}x^2\sqrt{x^2+1}=\int_0^{\frac{\hbar\Lambda}{\sqrt{4m\mu}}}\left(x^2+1\right)^{\frac{3}{2}}-\left(x^2+1\right)^{\frac{1}{2}}\,dx\\
=&\frac{1}{4}\left[x\left(x^2+1\right)^{\frac{3}{2}}-\frac{1}{2}x\left(x^2+1\right)^{\frac{1}{2}}-\frac{1}{2}\sinh^{-1}(x)\right]_0^{\frac{\hbar\Lambda}{4m\mu}}\\
=&\frac{1}{4}\left(\underbrace{\sqrt{1+x^{-2}}}_{=1+\frac{x^{-2}}{2}-\frac{x^{-4}}{4}+\mathcal{O}\left(x^{-6}\right)}x^2\left(x^2+1-\frac{1}{2}\right)-\frac{1}{2}\sinh^{-1}(x)\right)\Bigg|_{x=\frac{\hbar\Lambda}{\sqrt{4m\mu}}}\\
=&\frac{1}{4}\left(x^4+\left(\frac{1}{2}+\frac{1}{2}\right)x^2+\left(-\frac{1}{8}+\frac{1}{4}\right)+\mathcal{O}\left(x^{-2}\right)-\sinh^{-1}(x)\right)\Bigg|_{x=\frac{\hbar\Lambda}{\sqrt{4m\mu}}}
\end{aligned}
$$

is performed, which is again used in a secondary auxiliary calculation

$$\begin{aligned}
&\int_0^{\Lambda} k\frac{\hbar k}{\sqrt{2m}}\sqrt{\frac{\hbar^2k^2}{2m}+2\mu}\;dk\\
=&2\mu\left(\frac{\hbar^2}{4m\mu}\right)^{-1}\int_0^{\frac{\hbar\Lambda}{\sqrt{4m\mu}}} x^2\sqrt{x^2+1}\;dx\\
=&\frac{\hbar^2}{2m}\frac{\Lambda^4}{4}+\mu\frac{\Lambda^2}{2}+\frac{m\mu^2}{\hbar^2}\left(\frac{1}{4}-\sinh^{-1}\left(\frac{\hbar\Lambda}{\sqrt{4m\mu}}\right)\right)+\mathcal{O}\left(\Lambda^{-2}\right).
\end{aligned}$$

Inserting this auxiliary result and $n=2$ into the quantum fluctuations (3.107), yields

$$\begin{aligned}
&\sum_{k\neq 0}\frac{\sqrt{e_k(e_k+2\mu)}-\mu-e_k}{2}\\
\approx&\frac{L^2}{4\pi}\lim_{\Lambda\to\infty}\left(\frac{1}{4}\frac{\hbar^2}{2m}\Lambda^4+\frac{1}{2}\mu\Lambda^2+\frac{m\mu^2}{\hbar^2}\left(\frac{1}{4}-\sinh^{-1}\left(\frac{\hbar\Lambda}{\sqrt{4m\mu}}\right)\right)-\left[\frac{\hbar^2}{2m}\frac{k^4}{4}+\mu\frac{k^2}{2}\right]_0^{\Lambda}\right)\\
=&\frac{mL^2\mu^2}{4\pi\hbar^2}\left(\frac{1}{4}-\lim_{\Lambda\to\infty}\sinh^{-1}\left(\frac{\hbar\Lambda}{\sqrt{4m\mu}}\right)\right)\\
=&\frac{mL^2\mu^2}{4\pi\hbar^2}\left(\frac{1}{4}-\lim_{\Lambda\to\infty}\ln\left(\frac{\hbar\Lambda}{\sqrt{m\mu}}\right)\right).
\end{aligned}\tag{3.111}$$

In the last equality, the asymptotic form

$$\sinh^{-1}(x)=\ln(x+\sqrt{x^2+1})=\ln(2x)+\mathcal{O}\left(\frac{1}{x}\right)\tag{3.112}$$

was used.

Lastly, for the quantum fluctuations of the ground state occupation in two dimensions, the auxiliary calculation

$$\begin{aligned}
&\int_0^{\Lambda} k\frac{\frac{\hbar^2k^2}{4m\mu}+\frac{1}{4}}{\sqrt{\frac{\hbar^2k^2}{4m\mu}(\frac{\hbar^2k^2}{4m\mu}+1)}}\;dk\\
=&\;\frac{4m\mu}{\hbar^2}\int_0^{\frac{\hbar\Lambda}{2\sqrt{m\mu}}}\frac{x^2+\frac{1}{4}}{\sqrt{x^2+1}}\;dx\\
=&\;\frac{4m\mu}{\hbar^2}\int_0^{\frac{\hbar\Lambda}{2\sqrt{m\mu}}}\sqrt{x^2+1}-\frac{3}{4}\frac{1}{\sqrt{x^2+1}}\;dx\\
=&\;\frac{m\mu}{\hbar^2}\left[2x\sqrt{x^2+1}-\sinh^{-1}(x)\right]_0^{\frac{\hbar\Lambda}{2\sqrt{m\mu}}}\\
=&\;\frac{\Lambda^2}{2}+\frac{m\mu}{\hbar^2}\left(1-\ln\left(\frac{\hbar\Lambda}{\sqrt{m\mu}}\right)\right)+\mathcal{O}\left(\Lambda^{-1}\right)
\end{aligned}$$

is performed. By inserting this result and $n=2$ into the quantum fluctuations (3.108), one gets

$$\sum_{k\neq 0}\left(1-\frac{e_k+\frac{\mu}{2}}{\sqrt{e_k(e_k+2\mu)}}\right)\approx\frac{L^2m\mu}{2\pi\hbar^2}\lim_{\Lambda\to\infty}\ln\left(\frac{\hbar\Lambda}{e\sqrt{m\mu}}\right).\tag{3.113}$$

Regularization The preceding calculations are summarized. In the Green's function (3.102) and in the approximation (3.106) of the series by an integral, a parameter $\Lambda \in \mathbb{R}$ is introduced. A finite value of Λ corresponds to the integration over a sphere with that radius in momentum space and the limit $\lim_{\Lambda\to\infty}$ has to be formed to integrate over the entire space $\mathbb{R}^n$. The parameter Λ is passed down to the expressions (3.109), (3.110), (3.111) and (3.113) for the quantum fluctuations, as well as to the expression (3.105) for the inverse interaction strength. All of those expressions turn out to be divergent. Since the divergencies arise in the limit $\lim_{\Lambda\to\infty}$, they are called ultraviolet divergencies.

The process of introducing a finite value for Λ and postponing the limiting procedure is called cut-off regulariztion. Here, regularization refers to a more general set of heuristic procedures that aim at quantitatively describing diveregent expressions. The regularized quantum fluctuations and the regularized inverse interaction strength are inserted back into the ground state occupation (3.97) and into the super-canonical potential (3.98). It turns out, that each term in the mean-field contribution that would diverge with Λ is cancelled exactly by an according term in the quantum fluctuations. Then, performing the limit $\Lambda \to \infty$ afterwards yields the finite result

$$N_0 \approx -\sum_{k\in\frac{2\pi}{L}\mathbb{Z}^n\setminus 0} \frac{\mu+2e_k}{\sqrt{e_k(e_k+2\mu)}} \frac{1}{e^{\frac{\sqrt{e_k(e_k+2\mu)}+\hbar u\cdot k}{k_B T}}-1} - \frac{L^n m\mu}{2\pi\hbar^2} \begin{cases} -\frac{1}{2|a_s(0)|} + \frac{10}{3\pi}\frac{\sqrt{m\mu}}{\hbar} & n=3 \\ \ln\left(\frac{a_s(0)\sqrt{m\mu}}{2\hbar}\right) + 1 + \gamma & n=2 \end{cases} \tag{3.114}$$

for the ground state occupation and

$$\Omega \approx k_B T \sum_{k\neq 0} \ln\left(1 - e^{-\frac{\sqrt{e_k(e_k+2\mu)}+\hbar u\cdot k}{k_B T}}\right) + \frac{L^n m\mu^2}{4\pi\hbar^2} \begin{cases} -\frac{1}{2|a_s(0)|} + \frac{32}{15\pi}\frac{\sqrt{m\mu}}{\hbar} & n=3 \\ \ln\left(\frac{a_s(0)\sqrt{m\mu}}{2\hbar}\right) + \frac{1}{4} + \gamma & n=2 \end{cases} \tag{3.115}$$

for the super-canonical potential.

4 Classical thermodynamics

4.1 Spherical gas

An example of the thermodynamics of a Bose gas on a non-trivial manifold M, with a grand canonical description and without interaction is detailed out. The manifold of choice is the surface $M = \partial B_r(0)$ of a sphere with radius $r \in]0, \infty[$. On the one hand it is non-trivial in the sense that M is a two-dimensional sub-manifold of $\mathbb{R}^3$ and due to its non-zero curvature the Laplace-Beltrami operator is not a simple Laplace operator. On the other hand it is fairly easy to handle, as the eigenfunctions of the Laplace-Beltrami operator are well known and no boundary conditions have to be included since $\partial M = \{\}$.

First-quantized description The Laplace Beltrami operator on the surface M of a three-dimensional sphere parametrized in spherical coordinates is derived in Appendix C.3 and reads

$$\Delta = \frac{1}{r^2}\left(\frac{1}{\sin\vartheta_2}\frac{d^2}{d\vartheta_1^2} + \frac{1}{\sin(\vartheta_2)}\frac{d}{d\vartheta_2}\sin(\vartheta_2)\frac{d}{d\vartheta_2}\right). \tag{4.1}$$

The sperical harmonics Y_{lm_L} with indices/quantum numbers $l \in \mathbb{N}$ and $m_L \in \{-l \cdots l\}$ constitute a complete orthonormal set of solutions to its eigenvalue problem

$$\Delta Y_{lm_L}(\vartheta_1, \vartheta_2) = -\frac{l(l+1)}{r^2} Y_{lm_L}(\vartheta_1, \vartheta_2), \tag{4.2}$$

from which one reads out the energies

$$e_l = \frac{\hbar^2 l(l+1)}{2mr^2}. \tag{4.3}$$

Grand-canonical potential Inserting the set of quantum numbers $\nu = l$ and energies (4.3) of the sphere into the generic form (3.15) of the grand-canonical potential of a non-interacting gas on an arbitrary manifold yields

$$\Omega = k_\mathrm{B}T \sum_{l=0}^{\infty}\sum_{m=-l}^{l} \ln\left(1 - e^{-\frac{e_l-\mu}{k_\mathrm{B}T}}\right) = k_\mathrm{B}T \sum_{l=0}^{\infty}(2l+1)\ln\left(1 - e^{-\frac{\frac{\hbar^2 l(l+1)}{2mr^2}-\mu}{k_\mathrm{B}T}}\right), \tag{4.4}$$

where the summation over the quantum number m conviniently reduces to a factor $2l+1$ as the energies e_l only depend on the quantum number l. Since all energies $\varepsilon_\nu = e_l - \mu$ need to be positive due to the geometric series in equation (3.2), one finds the restriction

$$\mu < \inf_{l\in\mathbb{N}} e_l = e_0 = 0 \tag{4.5}$$

on the chemical potential. The grand-canonical potential is a function of the temperature T and of the chemical potential μ. It also depends on the surface area $V_\mathrm{2D} \equiv \int_M 1\, dx = 4\pi r^2$ of the sphere, which is interpreted as a two-dimensional generalization of a volume.

A small selection of relevant thermodynamical properties is investigated in more detail. First, the derivatives of first order of the grand-canonical potential are treated briefly. Due to Equation (A.16), the particle number can be retrieved from the grand-canonical potential via the derivative

$$N = -\left(\frac{\partial\Omega}{\partial\mu}\right)_{T,V_\mathrm{2D}} = \sum_{l=0}^{\infty} N_l. \tag{4.6}$$

Here, the occupation numbers N_l of the individual energy levels e_l

$$N_l = \frac{2l+1}{e^{\frac{e_l-\mu}{k_\mathrm{B}T}} - 1} \tag{4.7}$$

are introduced, consisting of a Bose-Einstein distribution $\frac{1}{e^{\frac{e_l-\mu}{k_\mathrm{B}T}}-1}$ with the multiplicity $2l+1$ of the respective energy level. Likewise, due to Equation (A.18), the entropy is given as

$$S = -\left(\frac{\partial\Omega}{\partial T}\right)_{V_{2D},\mu} = -k_B \sum_{l=0}^{\infty}(2l+1)\left(\ln\left(1-e^{-\frac{e_l-\mu}{k_B T}}\right) + \frac{e_l-\mu}{k_B T}\frac{1}{e^{\frac{e_l-\mu}{k_B T}}-1}\right). \tag{4.8}$$

Analogous to T and μ, the volume V_{2D} can be introduced in the model as a thermodynamical variable ab initio. This is unnecessarily complicated however, since chosing a fixed volume before constructing the probability space yields the same grand-canonical potential as including all homothetically scaled versions of the manifold in the sample space and imposing the constraints of fixed expectation value and zero variance of the volume afterwards. However, the latter approach does link the volume V_{2D} with its Lagrange multiplier $\frac{p_{2D}}{T}$ more clearly, where p_{2D} is a generalized pressure. Then, expressing the energies e_l in terms of the volume V_{2D} like $e_l = \frac{2\pi\hbar^2 l(l+1)}{mV_{2D}}$ allows to evaluated the generalized pressure through the derivative

$$p_{2D} \equiv -\left(\frac{\partial\Omega}{\partial V_{2D}}\right)_{\mu,T} = \frac{1}{V_{2D}}\sum_{l=0}^{\infty} e_l \frac{2l+1}{e^{\frac{e_l-\mu}{k_B T}}-1}. \tag{4.9}$$

Due to the energy E and the grand-canonical potential Ω being related through a Legendre transformation as in Equation (A.17), it holds

$$E = \Omega + TS + \mu N = \sum_{l=0}^{\infty} e_l \frac{2l+1}{e^{\frac{e_l-\mu}{k_B T}}-1}. \tag{4.10}$$

Comparing Equations (4.9) and (4.10) yields the simple realtion

$$E = p_{2D} V_{2D}. \tag{4.11}$$

Chemical potential In experimental setups, it is usually the particle number N that is dircetly controlable or measurable, rather than the chemical potential μ. Thermodynamic quantities are therefore more tangible and more useful, when expressed in terms of the set of variabes T, N and V_{2D}, instead of the set T, μ and V_{2D} which is provided naturally by the model. To this end, thermodynamic quantities dependent on T,N and μ are evaluated at the implicit function μ defined by

$$N(\mu(N,T,V_{2D}),T,V_{2D}) = N \tag{4.12}$$

From its definition follow the differentiation properties

$$\left(\frac{\partial\mu}{\partial T}\right)_{N,V_{2D}} = -\frac{\left(\frac{\partial N}{\partial T}\right)_{\mu,V_{2D}}}{\left(\frac{\partial N}{\partial \mu}\right)_{V_{2D},T}} \tag{4.13}$$

$$\wedge \quad \left(\frac{\partial\mu}{\partial V_{2D}}\right)_{T,N} = -\frac{\left(\frac{\partial N}{\partial V_{2D}}\right)_{T,\mu}}{\left(\frac{\partial N}{\partial \mu}\right)_{V_{2D},T}} \tag{4.14}$$

$$\wedge \quad \left(\frac{\partial\mu}{\partial N}\right)_{V_{2D},T} = \frac{1}{\left(\frac{\partial N}{\partial \mu}\right)_{V_{2D},T}}, \tag{4.15}$$

where sufficient differentiability is assumed.

Numerically, the value $\mu(N,T,V_{2D})$ of the chemical potential can be calculated as a zero of the function $N(\bullet,T,V_{2D}) - N$, where the series over the quantum number l in the function N is approximated by a partial sum. Alternatively, an approximate analytical result is found. The series over $l \in \mathbb{N}$ in (4.6) is construed as a trapezoidal sum, approximating the integration over $l \in]0,\infty[$, i.e.

$$N = \frac{N_0}{2} + \lim_{l\to\infty}\frac{N_l}{2} + \sum_{l=0}^{\infty}\frac{N_l + N_{l+1}}{2} \approx \frac{N_0}{2} + \int_0^{\infty} N_l \; dl. \tag{4.16}$$

Corrections to this approximation are given by the Euler-Maclaurin formula. Using $e_l = \frac{l(l+1)}{2}e_1$ the integrand N_l is expressed as a derivative, rendering the integration trivial:

$$\int_0^\infty N_l \, dl = \int_0^\infty \underbrace{(2l+1)}_{=\frac{2k_\mathrm{B}T}{e_1}\frac{d}{dl}\frac{e_l-\mu}{k_\mathrm{B}T}} \underbrace{\frac{1}{e^{\frac{e_l-\mu}{k_\mathrm{B}T}}-1}}_{=\frac{d}{dx}\ln\left(1-e^{-x}\right)|_{x=\frac{e_l-\mu}{k_\mathrm{B}T}}} dl$$

$$= \frac{2k_\mathrm{B}T}{e_1}\left[\ln\left(1-e^{-\frac{e_l-\mu}{k_\mathrm{B}T}}\right)\right]_{l=0}^{\infty}$$

$$= -\frac{2k_\mathrm{B}T}{e_1}\ln\left(1-e^{\frac{\mu}{k_\mathrm{B}T}}\right). \tag{4.17}$$

Consequently, the approximate analytical expression

$$N \approx \frac{1}{e^{-\frac{\mu}{k_\mathrm{B}T}}-1} - \frac{k_\mathrm{B}T}{e_1}\ln\left(1-e^{\frac{\mu}{k_\mathrm{B}T}}\right) \tag{4.18}$$

is found for the particle number. A more crude approximation involves a rectangular sum instead of the trapezoidal sum, resulting in the same expression for N except without the additive contribution $\frac{N_0}{2}$, which can then be solved for the chemical potential, yielding

$$\mu \approx k_\mathrm{B}T\ln\left(1-e^{-\frac{Ne_1}{2k_\mathrm{B}T}}\right). \tag{4.19}$$

Bose-Einstein condensation A phase transition occurs, when a derivative of the grand-canonical potential is discontinuous at some point along a path in the space of free parameters (an apropriate subset of the thermodynamic variables) of the system. More specifically, in the case of Bose-Einstein condensation, the heatcapacity (which is a second order derivative of the grand-canonical potential) has a discontinuity along a path of constant particle number and varying temperature. Such a phase transition is not present in the spherical gas of finite size. Nevertheless, another hallmark of Bose-Einstein condensation may be achieved, that is, the macroscopic occupation of the ground state. Here, ground state refers to the lowest energy single-particle state from the frist-quantized description. For the sphere, the ground state corresponds the quantum number $l = 0$. As there is no strict separation of phases, a criterion for the transition from "low" to "high" ground-state occupation is constructed.

The additive contribution of the quantum number $l = 0$ to the particle number N is the occupation number of the ground state and reads

$$N_0 = \frac{1}{e^{-\frac{\mu}{k_\mathrm{B}T}}-1}. \tag{4.20}$$

The occupation $N - N_0$ of the excited states is monotonically decreasing with both T and μ. For any given temperature the ground state occupation is therefore bounded from below by

$$N_0 = N - \sum_{l=1}^{\infty}\frac{2l+1}{e^{\frac{e_l-\mu}{k_\mathrm{B}T}}-1} \geq N - \sum_{l=1}^{\infty}\frac{2l+1}{e^{\frac{e_l}{k_\mathrm{B}T}}-1}. \tag{4.21}$$

It turns out that this bound is only larger than the trivial lower bound $N_0 \geq 0$ for temperatures smaller than a certain value T_c, at which it holds

$$N = \sum_{l=0}^{\infty}\frac{2l+1}{e^{\frac{e_l}{k_\mathrm{B}T_c}}-1}. \tag{4.22}$$

The temperature T_c is refered to as the critical temperature and is interpreted as the boundary between the regime of "low" ground state occupation ($T > T_c$) and "high" ground state occupation ($T < T_c$). Its value can be determined either numerically or analytically in analogy to the chemical potential. With a trapezoidal sum, the resulting analytic approximation reads

$$N \approx \frac{3}{2}\frac{1}{e^{-\frac{e_1}{k_\mathrm{B}T_c}}-1} - 2\frac{k_\mathrm{B}T_c}{e_1}\ln\left(1-e^{-\frac{e_1}{k_\mathrm{B}T_c}}\right). \tag{4.23}$$

The critical temperature, computed both from (4.22) and (4.23), is displayed in Figure 2, showing excellent agreement of the approximation with the exact result. Additionally, the trend of the critical temperature towards zero for increasing particle number N and radius r of the sphere is visible. This is in accordance with the Mermin-Wagner-Hohenberg theorem, which states, that in the thermodynamic limit, two-dimensional systems only exhibit Bose-Einstein condensation at zero temperature. Here, thermodynamic limit refers to the joined limit of infinite system size $R \to \infty$ and population $N \to \infty$, where the average particle density $\frac{V_{2D}}{N}$ approaches some finite limit.

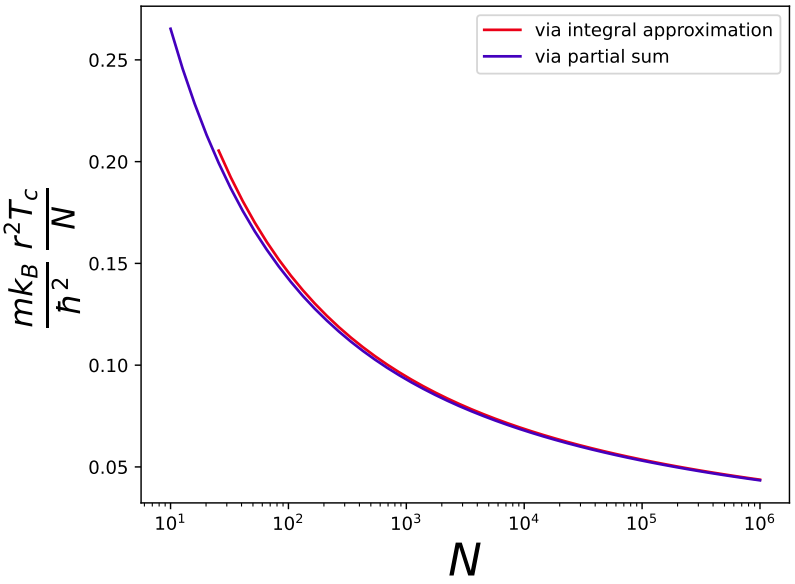


Figure 2: Critical temperature T_c of the spherical Bose gas as a as a function of the particle number N. Dependecies on any other system parameters are conveniently absorbed by the scaling factor of the vertical axis. The blue curve was generated by solving the exact expression (4.22) of the particle number for the critical temperature numerically, by approximating the series as a partial sum and solving for T_c with Newton's method. The red curve, on the other hand, stems from solving the analytic approximation (4.23) numerically via fixpoint iteration.

The now accessible critical temperature also provides a reasonable temperature range for plotting the ground-state occupation. Figure 3 shows the functional dependence of the groundstate occupation on the temperature, both for a small and for a large total particle number N. It can be seen that the actual ground state occupation approaches the lower bound for large occupation numbers, hinting at its convergence in the thermodynamic limit. Mind that this convergence removes the differentiability of the particle number at the critical temperature, thereby creating a true phase transition in the thermodynamic limit, which again is in accordance with the Mermin-Wagner-Hohenberg theorem.

Heat capacity As an example of a more involved thermodynamical quantity, the heat capacity is considered. The heat capacity at constant volume is defined as

$$c_V \equiv \left(\frac{\partial E}{\partial T}\right)_{N,V_{2D}}. \tag{4.24}$$

As discussed for the chemical potential, the modeling only provides an implicit dependence on the particle number, here $E(T, V_{2D}, \mu(T, V_{2D}, N))$. Therefore, with the chainrule and the derivative (4.13) of the implicit function μ with respect to T, the derivative is traced back to

$$\begin{aligned}\left(\frac{\partial E}{\partial T}\right)_{N,V_{2D}} &= \left(\frac{\partial E}{\partial T}\right)_{\mu,V_{2D}} + \left(\frac{\partial E}{\partial \mu}\right)_{V_{2D},T}\left(\frac{\partial \mu}{\partial T}\right)_{N,V_{2D}} \\ &= \left(\frac{\partial E}{\partial T}\right)_{\mu,V_{2D}} - \left(\frac{\partial E}{\partial \mu}\right)_{V_{2D},T}\frac{\left(\frac{\partial N}{\partial T}\right)_{V_{2D},\mu}}{\left(\frac{\partial N}{\partial \mu}\right)_{T,V_{2D}}}.\end{aligned} \tag{4.25}$$

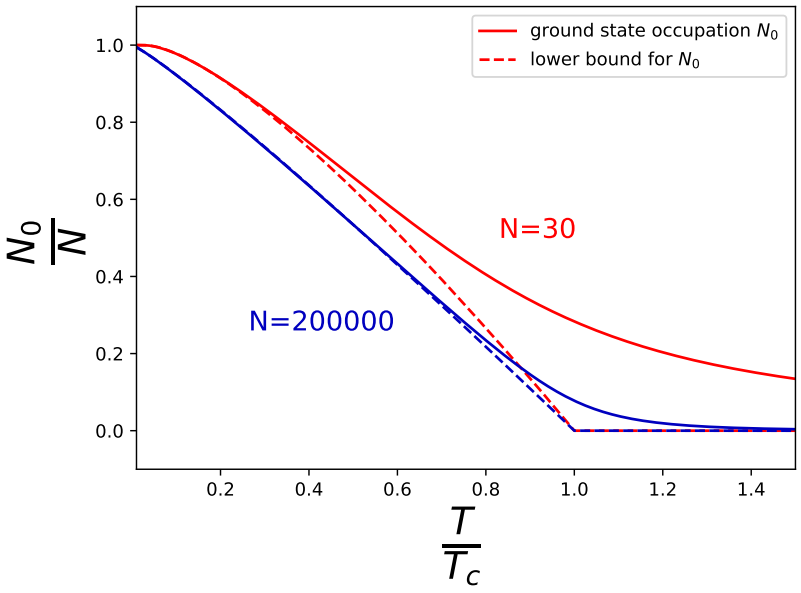


Figure 3: Ground state occupation N_0 in units of the respective total particle number N as a function of the temperature T in units of the respective critical temperature T_c. Continuous lines were generated by numerically evaluating (4.20) at the numerically determined chemical potential for each particle number. Dashed lines represent a lower bound for N_0, given by (4.21).

Expressions for the particle number N and the energy E as functions of the variables T,μ and $V_{2\mathrm{D}}$ are already known through Equations (4.6) and (4.10), respectively. Performing the four derivatives of E and N with respect to T and μ, and inserting everything back into (4.24) yields

$$4k_{\mathrm{B}}T^2c_V = \sum_{l=0}^{\infty} e_l^2 \frac{2l+1}{\sinh\left(\frac{e_l-\mu}{2k_{\mathrm{B}}T}\right)^2} - \frac{\left(\sum_{l=0}^{\infty} e_l \frac{2l+1}{\sinh\left(\frac{e_l-\mu}{2k_{\mathrm{B}}T}\right)^2}\right)^2}{\sum_{l=0}^{\infty} \frac{2l+1}{\sinh\left(\frac{e_l-\mu}{2k_{\mathrm{B}}T}\right)^2}}, \tag{4.26}$$

after small algebraic rearrangements. A simpler approximate expression for the heat capacity is derived in analogy to the treatment of the chemical potential. To this end, the three series $\sum_{l=0}^{\infty}$ in (4.26) are interpreted as rectangular sums approximating the integration $\int_0^{\infty} dl$. This, together with a consequent integration by substitution results in the auxiliary calculation

$$\begin{aligned}
&\sum_{l=0}^{\infty} e_l^n \frac{2l+1}{\sinh\left(\frac{e_l-\mu}{2k_{\mathrm{B}}T}\right)^2} \\
&\approx \int_0^{\infty} \underbrace{(2l+1)}_{=\frac{2k_{\mathrm{B}}T}{e_1}\frac{d}{dl}\frac{e_l-\mu}{k_{\mathrm{B}}T}} \quad \underbrace{e_l^n}_{=(k_{\mathrm{B}}Tx+\mu)^n|_{x=\frac{e_l-\mu}{k_{\mathrm{B}}T}}} \quad \underbrace{\sinh\left(\frac{e_l-\mu}{2k_{\mathrm{B}}T}\right)^{-2}}_{=\sinh\left(\frac{x}{2}\right)^{-2}|_{x=\frac{e_l-\mu}{k_{\mathrm{B}}T}}} dl \\
&= \frac{2k_{\mathrm{B}}T}{e_1} \int_{-\frac{\mu}{k_{\mathrm{B}}T}}^{\infty} (k_{\mathrm{B}}Tx+\mu)^n \sinh\left(\frac{x}{2}\right)^{-2} dx,
\end{aligned} \tag{4.27}$$

for any $n \in \{0,1,2\}$. Inserting these expressions back into (4.26) and simplifying yields

$$\frac{e_1}{2k_\mathrm{B}^2T}c_V \approx \int\limits_{-\frac{\mu}{k_\mathrm{B}T}}^{\infty} x^2 \sinh\left(\frac{x}{2}\right)^{-2}\, dl - \frac{\left(\int\limits_{-\frac{\mu}{k_\mathrm{B}T}}^{\infty} x \sinh\left(\frac{x}{2}\right)^{-2}\, dl\right)^2}{\int\limits_{-\frac{\mu}{k_\mathrm{B}T}}^{\infty} \sinh\left(\frac{x}{2}\right)^{-2}\, dl} \tag{4.28}$$

The antiderivatives of the integrands in (4.28) read

function	antiderivative
$\sinh\left(\frac{x}{2}\right)^{-2}$	$-\coth\left(\frac{x}{2}\right)$
$x\sinh\left(\frac{x}{2}\right)^{-2}$	$-x\coth\left(\frac{x}{2}\right) + 2\ln\left(\sinh\left(\frac{x}{2}\right)\right)$
$x^2\sinh\left(\frac{x}{2}\right)^{-2}$	$-x^2\left(1+\coth\left(\frac{x}{2}\right)\right) + 4x\ln\left(2\sinh\left(\frac{x}{2}\right)\right) - 4\mathrm{Li}_2\left(e^{-x}\right)$

Here Li_2 denotes the dilogarithm. Therewith solving the integrals and perfoming some algebraic rearrangements, one ends up with the simplified analytical expression

$$\frac{e_1}{4k_\mathrm{B}^2T}c_V \approx \mathrm{Li}_2\left(e^{\frac{\mu}{k_\mathrm{B}T}}\right) - \frac{\ln\left(1-e^{\frac{\mu}{k_\mathrm{B}T}}\right)^2}{\coth\left(\frac{x}{2}\right)-1} \tag{4.29}$$

for the heat capacity. Lastly, to return to the more intuitive set of variables T,N and V_2D, the approximation of the heat capacity (4.29) is evaluated at the approximated chemical potential (4.19), yielding

$$\frac{c_V}{Nk_\mathrm{B}} \approx \left(\mathrm{Li}_2\left(1-e^{-x}\right) - \frac{x}{e^x-1}\right)\bigg|_{x=\frac{2k_\mathrm{B}T}{Ne_1}}. \tag{4.30}$$

Interestingly, the approximate expression for the specific heat capacity (4.30) only depends on one parameter combining all three variables, which is not evident for the exact expression (4.26). Figure 4 shows the functional dependence of the exact expression (4.26) of heat capacity alongside the approximation (4.30) of the heat capacity. A good agreement between the exact numerical result and the approximate anayltical result is visible, which becomes better for higher particle number. Furthermore, the behaviour of the heat capacity in the limit of small and large temperatures is clearly visible, going to zero with $T \to 0$ and towards k_B in the limit $T \to \infty$.

Compressibility The compressibility at constant temperature is defined as

$$\kappa_T = -\frac{1}{V_\mathrm{2D}}\left(\frac{\partial V_\mathrm{2D}}{\partial p}\right)_{T,N}. \tag{4.31}$$

It is treated analogously to the heat capacity, but the implicit dependencies are slightly more intricate: First, the volume as a function V_2D of p_2D,T and N is related to the pressure as a function p'_2D of V_2D, T and N as the implicit function defined by $p'_\mathrm{2D}(T,N,V_\mathrm{2D}(T,N,p_\mathrm{2D})) = p_\mathrm{2D}$. From the definition of the function V_2D follows the differentiation property

$$\left(\frac{\partial V_\mathrm{2D}}{\partial p_\mathrm{2D}}\right)_{T,N} = \frac{1}{\left(\frac{\partial p'_\mathrm{2D}}{\partial V_\mathrm{2D}}\right)_{T,N}}. \tag{4.32}$$

Second, the pressure as a function p'_2D of T, V_2D and N is related to the pressure as a function p_2D of T, V_2D and μ through the implicit function μ via $p'_\mathrm{2D}(T,V_\mathrm{2D},N) \equiv p_\mathrm{2D}(T,V_\mathrm{2D},\mu(T,V_\mathrm{2D},N)$. Using the chainrule and the derivative (4.13) of μ with respect to V_2D one gets

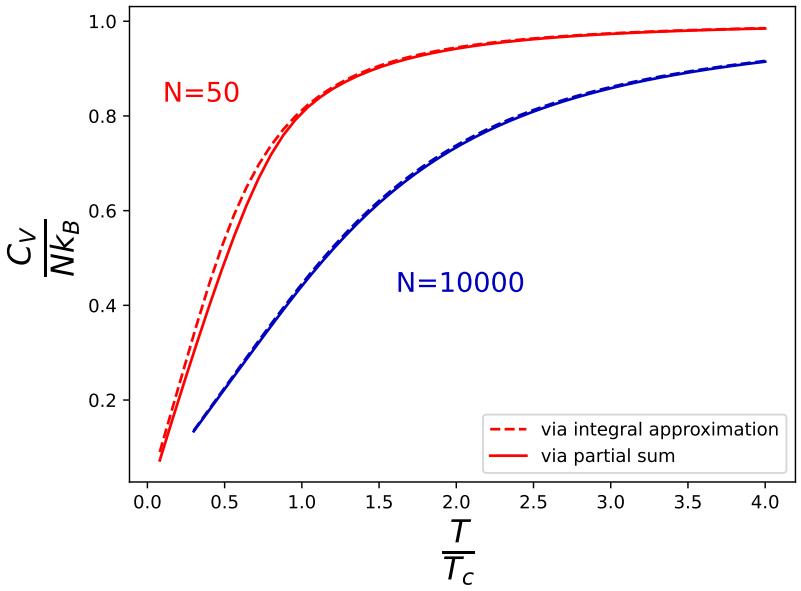


Figure 4: Specific heat capacity $\frac{c_V}{N}$ of a spherical bose Gas in units of the Boltzmann constant k_B as a function of the temperature T in units of the respective critical temperature T_c for different total particle numbers N. Solid lines were generated by numerically evaluating (4.26) at the numerically evaluated chemical potential. Dashed lines stem from evaluating the simplified analytical approximation (4.30) of the heat capacity.

$$\begin{aligned}\left(\frac{\partial p_{2\mathrm{D}}}{\partial V_{2\mathrm{D}}}\right)_{T,N} &= \left(\frac{\partial p_{2\mathrm{D}}}{\partial V_{2\mathrm{D}}}\right)_{T,\mu} + \left(\frac{\partial p_{2\mathrm{D}}}{\partial \mu}\right)_{V_{2\mathrm{D}},T}\left(\frac{\partial \mu}{\partial V_{2\mathrm{D}}}\right)_{T,N} \\ &= \left(\frac{\partial p_{2\mathrm{D}}}{\partial V_{2\mathrm{D}}}\right)_{T,\mu} - \left(\frac{\partial p_{2\mathrm{D}}}{\partial \mu}\right)_{V_{2\mathrm{D}},T}\frac{\left(\frac{\partial N}{\partial V_{2\mathrm{D}}}\right)_{T,\mu}}{\left(\frac{\partial N}{\partial \mu}\right)_{V_{2\mathrm{D}},T}}.\end{aligned} \tag{4.33}$$

Evaluating the four derivatives of the pressure (4.9) and the particle number (4.6) with respect to $V_{2\mathrm{D}}$ and μ, inserting them back into (4.33) and performing some algebraic rearrangements yields

$$4k_\mathrm{B}T\frac{V_{2\mathrm{D}}}{\kappa_T} = -\sum_{l=0}^{\infty} e_l^2 \frac{2l+1}{\sinh\left(\frac{e_l-\mu}{2k_\mathrm{B}T}\right)^2} + \frac{\left(\sum_{l=0}^{\infty} e_l \frac{2l+1}{\sinh\left(\frac{e_l-\mu}{2k_\mathrm{B}T}\right)^2}\right)^2}{\sum_{l=0}^{\infty}\frac{2l+1}{\sinh\left(\frac{e_l-\mu}{2k_\mathrm{B}T}\right)^2}} - 8k_\mathrm{B}T\sum_{l=0}^{\infty} e_l \frac{2l+1}{e^{\frac{e_l-\mu}{k_\mathrm{B}T}}-1}. \tag{4.34}$$

A comparison of the expression (4.34) for the compressibiliy with the expressions (4.26) for the heat capacity and (4.10) for the energy reveals the surprisingly simple relation

$$Tc_V + \frac{V_{2\mathrm{D}}}{\kappa_T} = 2E. \tag{4.35}$$

4.2 Two dimensional box

The classical themodynamics of the interacting Bose gas in a two-dimensional box with a super-canonical description is set up in section 3.2. There, the expression

$$\Omega \approx -\frac{L^2 m\mu^2}{4\pi\hbar^2}\left(\ln\left(\frac{2\hbar}{a_s(0)\sqrt{m\mu}}\right) - \frac{1}{4} - \gamma\right) + k_B T\sum_{k\neq 0}\ln\left(1 - e^{-\frac{\sqrt{e_k(e_k+2\mu)}+\hbar u\cdot k}{k_B T}}\right) \tag{4.36}$$

is derived for the super-canonical potential in equation (3.115). The particle number is immediately accessible through a derivative with respect to the chemical potential, i.e.

$$N = -\frac{d\Omega}{d\mu} = -\frac{L^2 m\mu}{2\pi\hbar^2}\left(\ln\left(\frac{a_s(0)\sqrt{m\mu}}{2\hbar}\right) + \frac{3}{4} + \gamma\right) - \sum_{k\neq 0} \frac{2e_k}{\sqrt{e_k(e_k+2\mu)}} \frac{1}{e^{\frac{\sqrt{e_k(e_k+2\mu)}+\hbar u\cdot k}{k_B T}} - 1}. \tag{4.37}$$

Comparing the total particle number (4.37) with the ground state occupation number N_0

$$N_0 = -\frac{L^2 m\mu}{2\pi\hbar^2}\left(\ln\left(\frac{a_s(0)\sqrt{m\mu}}{2\hbar}\right) + 1 + \gamma\right) - \sum_{k\neq 0} \frac{\mu + 2e_k}{\sqrt{e_k(e_k+2\mu)}} \frac{1}{e^{\frac{\sqrt{e_k(e_k+2\mu)}+\hbar u\cdot k}{k_B T}} - 1} \tag{4.38}$$

from equation (3.114) at zero temperature yields the non-zero condensate depletion

$$(N - N_0)|_{T=0} = \frac{L^2 m\mu}{8\pi\hbar^2}, \tag{4.39}$$

meaning that the Bose gas never fully condenses, even for minimal thermal fluctuations.

It remains to demonstrate, that the additional constraint of fixing the system's momentum p, introduced in the super-canonical ensemble, leads to the emergence of the phenomenon of superfluidity in the classical thermodynamics. The momentum p is related to the velocity u by

$$p = -\nabla_u \Omega, \tag{4.40}$$

due to Equation (A.16). In the following, the behaviour of p for small velocities u is investigated. Only the thermal fluctuations of the super-canonical potential Ω depend on u and are expanded into the Taylor polynomial

$$\ln(1 - e^{-(x_0+x)}) = \ln(1 - e^{-x_0}) + \frac{1}{e^{x_0} - 1}\frac{x}{1!} - \frac{e^{x_0}}{(e^{x_0}-1)^2}\frac{x^2}{2!} + \mathcal{O}\left(x^3\right) \tag{4.41}$$

evaluated at $x_0 = \frac{\sqrt{e_k(e_k+2\mu)}}{k_B T}$ and $x = \frac{\hbar u\cdot k}{k_B T}$. The terms of first and second order in x are simplified with the following auxiliary considerations. The set $\frac{2\pi}{L}\mathbb{Z}^2$ of quantum numbers is invariant under interchanging and changing the sign of its components, leading to the identities

$$\sum_{k\neq 0} k \cdots (\|k\|) = \sum_{k\neq 0} -k \cdots (\|k\|) = 0 \tag{4.42}$$

and

$$i \neq j \Rightarrow \sum_{k\neq 0} k_i k_j \cdots (\|k\|) = \sum_{k\neq 0} -k_i k_j \cdots (\|k\|) = 0, \tag{4.43}$$

which in turn yield the secondary auxiliary results

$$\sum_{k\neq 0} u\cdot k \cdots (\|k\|) = \sum_{i=1}^{2} u_i \sum_{k\neq 0} k_i \cdots (\|k\|) = 0 \tag{4.44}$$

and

$$\sum_{k\neq 0} (u\cdot k)^2 \cdots (\|k\|) = \sum_{i=1}^{2} u_i^2 \sum_{k\neq 0} k_i^2 \cdots (\|k\|) = \|u\|^2 \sum_{k\neq 0} \|k\|^2 \cdots (\|k\|). \tag{4.45}$$

Therewith, the thermal fluctuations take the form

$$k_B T \sum_{k\neq 0} \ln\left(1 - e^{-\frac{\sqrt{e_k(e_k+2\mu)}+\hbar u\cdot k}{k_B T}}\right) = k_B T \sum_{k\neq 0} \ln\left(1 - e^{-\frac{\sqrt{e_k(e_k+2\mu)}}{k_B T}}\right) \tag{4.46}$$

$$- \frac{m\|u\|^2}{2} \sum_{k\neq 0} \frac{e_k}{k_{\mathrm{B}} T} \frac{e^{-\frac{\sqrt{e_k(e_k+2\mu)}}{k_B T}}}{\left(e^{-\frac{\sqrt{e_k(e_k+2\mu)}}{k_B T}} - 1\right)^2} + \mathcal{O}\left(\|u\|^3\right). \tag{4.47}$$

Consequently, inserting (4.46) into (4.36) and performing the derivative (4.40), yields the expression

$$p = -\nabla_u \Omega = mu \underbrace{\sum_{k\neq 0} \frac{e_k}{k_{\mathrm{B}} T} \frac{e^{-\frac{\sqrt{e_k(e_k+2\mu)}}{k_B T}}}{\left(e^{-\frac{\sqrt{e_k(e_k+2\mu)}}{k_B T}} - 1\right)^2}}_{\equiv N_{\mathrm{n}}} + \mathcal{O}\left(\|u\|^2\right). \tag{4.48}$$

for the momentum. For small u, the momentum is approximately proportional to the velocity u, analogous to the momentum of a cloud of N_n classical particles of mass m moving at the avearge velocity u. Intriguingly, the particle number N_n, called the normal fluid particle number, differs from the total particle number N by the so-called superfluid particle number $N_{\mathrm{s}} \equiv N - N_0$. The momentum (4.48) is rewritten as

$$p = m(uN_{\mathrm{n}} + 0N_{\mathrm{s}}), \tag{4.49}$$

suggesting that the gas can be decomposed into two components, one of which complies with the externally imposed non-zero momentum by moving at an average velocity u (the normal fluid), while the other is unmoved and apparently frictionless, as it does not get dragged along with the rest (the super fluid). This idea of a two-fluid model dates back to 1941 and was introduced by Lew Landau [16]. The superfluid occupation number N_s also differs from the ground state occupation number, thereby showcasing that superfluidity and Bose-Einstein condensation are indeed distinct phenomena.

5 Conclusion

5.1 Summary

The main achievements of the thesis are summarized.

Statistical mechanics is construed as a compound model combining microscopic physics and statistics. The statistical model of ensemble theory is provided with an intuitive interpretation in section 2.2 and is given a mathematical framework based on the concepts of probability theory in appendix A. With the gained insights, the grand canonical ensemble is successfully extended to include superfluidity (at least for the Bose gas in a box), as can be seen by the emergence of a shadow of Landau's two fluid model in the resulting classical themodynamics in section 4.2.

Bogoliubov's [17] original theory for including interactions in the quantum statistical treatment of a Bose gas in a three-dimensional box with periodic boundary conditions is successfully generalized to work on arbitrary (sufficiently differnetiabel) manifolds in section 3.1 (given that solutions to the eigenvalue problem of the Laplace-Beltrami operator of that geometry are known). The involved differential geometry is derived in an intuitive manner in appendix C.

The heuristic cutoff regularization applied in 3.2 to remove ultraviolet divergencies in the mean field contributions and quantum fluctuations is given a mathematical basis by the coarse graining scheme proposed in appendix E.

Some smaller achievements include solving and probabilistically interpreting the scattering theory both in two and three dimensions in appendix D, the intuitive derivation of the functional derivative based on generalized directional derivatives as an alternative to heuristic variational techniques in appendix B, the classical thermodynamical treatment of the non-interacting Bose gas on the surface of a sphere (in particular the rigorous treatment of implicit dependencies) in section 4.1, as well as the attempt of intuitively deriving the density operator formalism of quantum statistics in appendix A.3.

5.2 Outlook

A set of flaws of the current state of the thesis should be pointed out that might deserve future investigation. First, the grand- and super-canonical ensemble allow for fluctuations in the particle number, which is not a good model for typical trapped atomic gases, especially for a low number of atoms. Second, in the treatment of the Bose gas in a box, periodic boundary conditions are assumed, while typical experimental setups rather provide Dirichlet boundary conditions. Including these into the formalism proves to be non-trivial however, as the technical requirement on an adequate basis of eigenfunctions of the Laplace Beltrami operator compliant with Dirichlet boundary conditions does not exist. Furthermore, including superfluidity analogously to the box on other geometries seems difficult. For the high symmetry manifold that is the surface of a sphere, superfluidity may be included by exchanging the constraint of fixing the expectation value of the system's momentum with fixing the angular momentum, since the spherical harmonics are simultaneous eigenfunctions of the Laplace-Beltrami operator and of the angular momentum operator. Third, approximating a general interaction potential by contact interaction collapses all its complexity into a single number. Especially for unisotropic interactions, this approximation extinguishes important physical aspects. Fourth, an additional layer of complexity may be added to the formalism by including a more realistic mean field obeying the Gross-Pitaevski equation, such that vortex physics enters the picture.

A Probability theory of equilibrium ensembles

Probability spaces Probability spaces are a mathematical construct designed for the rigorous treatment of the concepts of "uncertainty" ,"probability" or "chance". They come in the shape of a triplet $(\Omega, \mathcal{A}, \mathbb{P})$, where Ω denotes the sample space, $\mathcal{A} \subseteq \mathbb{P}(\Omega)$ the event space and $\mathbb{P} : \mathcal{A} \to [0, 1]$ the probability measure. By construction, $\mathbb{P}(A)$ is to be interpreted as the probability that one of the samples $\omega \in A$ occured for any given $A \in \mathcal{A}$. (Both A and $\mathbb{P}$ must have certain elementary properties that aren't listed here).

A.1 Entropy

Entropy is an elaborated attempt of condensing the "total amount of uncertainty" of a probability space – encapsulated mainly in its probability measure – into a single real number. A short intuitive derivation is given.

Surprisal of an event One starts by constructing a function s that associates to each event $A \in \mathcal{A}$ the "surprisal" or synonymously the "amount of information gained" upon its incidence. Three properties of s are postulated that uniquely define it. First, the function should only depend on $\mathbb{P}(A)$, not on A itself, i.e.

$$\begin{aligned} s &= \sigma \circ \mathbb{P} \\ \sigma &:]0, 1] \to \mathbb{R}. \end{aligned} \tag{A.1}$$

Secondly one postulates, that if two stochastically independent events occur simultaneously, the sum of their individual information is gained:

$$\forall A, A' \in \mathcal{A} : \quad \mathbb{P}(A \cap A') = \mathbb{P}(A)\mathbb{P}(A') \Rightarrow s(A \cap A') = s(A) + s(A'). \tag{A.2}$$

This condition is fulfilled iff $\sigma \propto \ln$ as it is the unique solution to the functional equation $\sigma(xy) = \sigma(x) + \sigma(y)$. One already reads off the intuitive result, that the incidence of safe events does not hold any surprisal. Third, one requires, that the occurence of events with higher probability holds less surprisal

$$\mathbb{P}(A) > \mathbb{P}(A') \Rightarrow s(A) < s(A'). \tag{A.3}$$

Therefore, a negative proportionality constant has to be chosen in σ, where the absolute value is still a free parameter. In the application to physics, the convention is to choose the negative Boltzmann constant. Then, the final result for σ reads

$$\sigma = -k_{\mathrm{B}} \ln . \tag{A.4}$$

Expected surprisal of a $\mathbb{P}$-almost partition The next step is to define the "expected surprisal" of certain sets of events, the so-called $\mathbb{P}$-quasi partitions of $\mathcal{A}$. A $\mathbb{P}$-quasi partition $a \subseteq \mathcal{A}$ is a finite set of events, such that always exactly one of the events comprised in it occures almost surely, which can be mathematically formulated as

$$\begin{aligned} &\mathbb{P}\left(\bigcup_{A \in a} A\right) = 1 \\ \wedge \quad &\forall A, A' \in \mathcal{A} : A \neq A' \Rightarrow \mathbb{P}(A \cap A') = 0. \end{aligned} \tag{A.5}$$

This definition constitutes a slight relaxation of the usual definition of a partition, that allows for the intersections to be null sets instead of only the empty set. For such a set a the expected surprisal $\mathcal{S}(a)$ is defined intuitively as the sum over all $A \in a$ of the individual surprisals $s(A)$ weighted with the respective probabilities $\mathbb{P}(A)$, i.e.

$$\mathcal{S}(a) \equiv \sum_{A \in a} s(A)\mathbb{P}(A). \tag{A.6}$$

Entropy of a probability space Finally, the entropy of the probability space is defined as the supremum of the expected surprisal over all $\mathbb{P}$-quasi partitions of $\mathcal{A}$:

$$S \equiv \sup_{\substack{a \subseteq \mathcal{A} \\ \mathbb{P}-\text{quasi partition}}} \mathcal{S}(a). \tag{A.7}$$

A $\mathbb{P}$-almost partition a' is called a $\mathbb{P}$-almost refinement of another $\mathbb{P}$-almost partition a, iff all sets in a' are subsets of sets in a apart from nullsets, i.e. $\forall A' \in a' \exists A \in a : \mathbb{P}(A' \setminus A) = 0$. This definition constitutes a relaxation of the common definition of the refinement of a partition. As the expected surprisal of a $\mathbb{P}$-almost partition is monotonically increasing under $\mathbb{P}$-almost refinement, taking the supremum can be interpreted as regarding ever-finer getting $\mathbb{P}$-almost partitions.

To give an example, the most trivial case of a probability space with finite sample space $\Omega = \{1, \cdots N\}$ is considered, where $N \in \mathbb{N}$. Then the set $\{\{1\}, \cdots \{N\}\}$ constitutes a $\mathbb{P}$-almost partition, irrespective of the probability measure $\mathbb{P}$. Furthermore, it is also a $\mathbb{P}$-almost refinement of any other $\mathbb{P}$-almost partition. Consequently the entropy of the probability space evaluates to the familar result

$$S = \mathcal{S}(\{\{1\}, \cdots \{N\}\}) = -k_\mathrm{B} \sum_{\omega=1}^{N} \ln\left(\mathbb{P}(\{\omega\})\right) \mathbb{P}(\{\omega\}). \tag{A.8}$$

For a certain class of probability spaces that are generalizations of the previous example, the entropy can be stated explicitly. Assume, that the probability measure of any measurable set A is expressible as an integral with respect to some measure p of a measurable function $\tilde{\mathbb{P}} : \Omega \to [0, \infty[$ over A i.e.

$$\mathbb{P}(A) = \int_A \tilde{\mathbb{P}} \, dp. \tag{A.9}$$

The function $\tilde{\mathbb{P}}$ is a random variable, called the density of the probability measure $\mathbb{P}$ with respect to the measure p. The random variables form a vector space, when equipped with pointwise addition and multiplication. Then, the integration allows for the definition of a bilinear form $\langle \bullet, \bullet \rangle = \int \bullet \bullet \, dp$, which is further assumed to be a scalar product. In this setting, the expectation value of any random variable $\tilde{x}$ is expressible as

$$\mathbb{E}(\tilde{x}) = \int_\Omega \tilde{x}\tilde{\mathbb{P}} \, dp = \langle \tilde{x}, \tilde{\mathbb{P}} \rangle, \tag{A.10}$$

if it exists. In particular, the entropy turns out to be the expectation value of the random variable $\sigma \circ \tilde{\mathbb{P}}$, i.e.

$$S = \mathbb{E}(\sigma \circ \tilde{\mathbb{P}}) = \langle \sigma \circ \tilde{\mathbb{P}}, \tilde{\mathbb{P}} \rangle. \tag{A.11}$$

Probability spaces, for which the probability measure has a density, are the most commonly used class of probability spaces. A small set of examples is listed in Table A.1.

Ω	$\mathcal{A}$	p	$\int_A \bullet \, dp$		application in physics
$\subset \mathbb{N}$ finite	$\mathcal{P}(\Omega)$	counting measure	$\sum_{\omega \in \Omega} \bullet(\omega)$	sum	
$\widehat{=}\mathbb{N}$	$\mathcal{P}(\Omega)$	counting measure	$\sum_{\omega \in \Omega} \bullet(\omega)$	series	quantum statistics
$\subseteq \mathbb{R}^n$	$\mathcal{B}(\Omega)$	Lebesgue measure	$\int_{\omega \in \Omega} \bullet(\omega) \, d\omega$	Riemann integral	classical statistics
$\widehat{=}\mathbb{R}^\mathbb{N}$			$\int_{\omega \in \Omega} \bullet(\omega) \, \mathcal{D}\omega$	functional integral	

Table 4: Common examples of probability spaces $(\Omega, \mathcal{A}, \mathbb{P})$, where the probability measure $\mathbb{P}$ has a density $\tilde{\mathbb{P}}$ with respect to some measure p. Each subsequent row represents a more complex configuration, that arises from the previous one in some limiting case. ($\mathcal{P}$ and $\mathcal{B}$ denote the power set and the Borel σ-algebra, respectively).

A.2 Ensemble theory

An (equilibrium) ensemble is a probability space, constructed by equipping a measurable space $(\Omega, \mathcal{A})$ with the probability measure $\mathbb{P}$ that extremizes its entropy. In this setting, the entropy is to be viewed as a functional of the probability measure. The extremization of S with respect to $\mathbb{P}$ is performed by setting the functional derivative to zero, i.e. $\frac{\delta S}{\delta \mathbb{P}} \stackrel{!}{=} 0$.

Additionally, the extremization may be conducted compliant with certain constraints, fixing the expectation value of a random vector $\tilde{X} : \Omega \to \mathbb{R}^n$ to some vector $X \in \mathbb{R}^n$, i.e. $\mathbb{E}(\tilde{X}) \stackrel{!}{=} X$. The compliance with these constraints is then built into the extremization by introducing a vector $\Lambda \in \mathbb{R}^n$ of Lagrange multipliers. One particular additional constraint, that always has to be included to ensure that $\mathbb{P}$ is a probability measure is $\mathbb{E}(1) = \mathbb{P}(\Omega) = 1$, where the corresponding Lagrange multiplier is denoted by λ. (The Lagrange multipliers are dependent on the choice of X but the functional dependence is ommited in the notation). That way, the extremization compliant with constraints can be achieved by setting

$$0 \stackrel{!}{=} \frac{\delta\ S + (\mathbb{E}(1) - 1)\lambda + (\mathbb{E}(\tilde{X}) - X) \cdot \Lambda}{\delta \mathbb{P}}. \tag{A.12}$$

Assume now, that the entropy-extremizing probability measure possesses a density. Then the entropy is expressible as (A.11) and the expectation values are expressible as scalar products. Consequently the functional derivative can be evaluated following the considerations in appendix B, using in particular the linearity of the functional derivative and Equation (B.4), yielding

$$\begin{aligned}
0 &= \frac{\delta}{\delta \mathbb{P}} \left(S + (\mathbb{E}(1) - 1)\lambda + (\mathbb{E}(\tilde{X}) - X) \cdot \Lambda \right) \\
&= \frac{\delta}{\delta \mathbb{P}} \left(\mathbb{E}(\sigma \circ \tilde{\mathbb{P}} + \lambda + \tilde{X} \cdot \Lambda) - (\lambda + X \cdot \Lambda) \right) \\
&= \frac{\delta}{\delta \mathbb{P}} \langle \sigma \circ \tilde{\mathbb{P}} + \lambda + \tilde{X} \cdot \Lambda, \tilde{\mathbb{P}} \rangle \\
&= \underbrace{\frac{d \cdot \sigma(\cdot)}{dz} \circ \tilde{\mathbb{P}}}_{= -k_\mathrm{B}(\ln \circ \tilde{\mathbb{P}} + 1)} + \lambda + \tilde{X} \cdot \Lambda \\
\Leftrightarrow \tilde{\mathbb{P}} &= \underbrace{e^{\frac{\lambda}{k_\mathrm{B}} - 1}}_{\equiv \frac{1}{Z}} e^{\frac{1}{k_\mathrm{B}} \Lambda \cdot \tilde{X}},
\end{aligned} \tag{A.13}$$

where the partition function Z is introduced. Due to the constraint $\mathbb{E}(1) = 1$ one gets $Z = \left\langle 1, e^{\frac{1}{k_\mathrm{B}} \Lambda \cdot \tilde{X}} \right\rangle$. Therefore it follows for the other constraints

$$X = \mathbb{E}(\tilde{X}) = \langle \tilde{X}, \tilde{\mathbb{P}} \rangle = \frac{1}{Z} \left\langle \tilde{X}, e^{\frac{1}{k_\mathrm{B}} \Lambda \cdot \tilde{X}} \right\rangle = \frac{1}{Z} \left\langle 1, \tilde{X} e^{\frac{1}{k_\mathrm{B}} \Lambda \cdot \tilde{X}} \right\rangle = \frac{1}{Z} k_\mathrm{B} \nabla_\Lambda Z = \nabla_\Lambda k_\mathrm{B} \ln(Z). \tag{A.14}$$

Finally the extremized entropy can be expressed as a function of the chosen expectation values X (or rather implicitly of the Lagrange multipliers Λ) as

$$S = \mathbb{E}(\sigma \circ \tilde{\mathbb{P}}) = -k_\mathrm{B} \mathbb{E} \left(\ln \circ \left(\frac{1}{Z} e^{\frac{1}{k_\mathrm{B}} \Lambda \cdot \tilde{X}} \right) \right) = k_\mathrm{B} \ln(Z) - \Lambda \cdot X. \tag{A.15}$$

In conjunction Equations (A.14) and (A.15) mean that the entropy S is a Legendre transformation of the potential $k_\mathrm{B} \ln(Z)$, with respect to all Lagrange mulipliers Λ.

Application to physics In the application to physics, usually the expectation value of the random variable $\tilde{E}$ corresponding to the energy of the system is fixed to some value $E \in \mathbb{R}$. The according Lagrange multiplier is written as $-\frac{1}{T}$, where $T \in [0, \infty[$ is labeled the temperature of the system. The non-negativity of the temperature is usually needed to assure convergence of the partition function Z, since the energies of the microstates are usually bounded from below but not from above. The Lagrange multipliers corresponding to the other random variables $\tilde{X}$ are also expressed in the form $\Lambda = \frac{\Lambda'}{T}$. Under these conditions Equation (A.14) changes to

$$X = \nabla_{\Lambda'} k_\mathrm{B} T \ln(Z), \tag{A.16}$$

while Equation (A.15) is rearranged into

$$E = -k_{\mathrm{B}} T \ln(Z) + TS + \Lambda' \cdot X. \tag{A.17}$$

In essence, this kind of reparametrization of the Lagrange multipliers exchanges the roles of the energy and of the entropy. By evaluating the derivative

$$\begin{aligned}
\frac{d}{dT} k_{\mathrm{B}} T \ln(Z) &= k_{\mathrm{B}} \ln(Z) + k_{\mathrm{B}} T \frac{1}{Z} \frac{d}{dT} \left\langle 1, e^{-\frac{1}{k_{\mathrm{B}} T}(\tilde{E} - \Lambda' \cdot \tilde{X})} \right\rangle \\
&= k_{\mathrm{B}} \ln(Z) + k_{\mathrm{B}} T \left\langle \frac{1}{k_{\mathrm{B}} T^2}(\tilde{E} - \Lambda' \cdot \tilde{X}), \frac{1}{Z} e^{-\frac{1}{k_{\mathrm{B}} T}(\tilde{E} - \Lambda' \cdot \tilde{X})} \right\rangle \\
&= k_{\mathrm{B}} \ln(Z) + \frac{1}{T}(E - \Lambda' \cdot X)
\end{aligned}$$

and comparing with Equation (A.17), it is revealed, that now the entropy may be expressed as the derivative

$$S = \frac{d}{dT} k_{\mathrm{B}} T \ln(Z). \tag{A.18}$$

In conjunction, Equations (A.16), (A.18) and (A.17) mean that the energy of the system is a Legendre transformation of the quantity $-k_{\mathrm{B}} T \ln(Z)$ with respect to the temperature T and all Lagrange multipliers Λ'.

A.3 Quantum statistics

A statistical model of an experimental setup probing a quantum systems has to include two distinct sources of uncertainty. The usual uncertainty about the exact microstate of the observed system is accompanied by an additional randomness due to the uncertainty of the effect that a measurement has on the system. In the following, these two types of uncertainty are treated separately first and merged into a unified statistical description afterwards.

Unperturbed system The set of possible states of an unperturbed system is usually assumed to be given by a separable Hilbert space $\mathcal{H}$. A statistical model of the uncertainty of the microscopic state of the system then naturally involves a probability space with sample space $\mathcal{H}$, where the probability measure is postulated to be of the form

$$\mathbb{P}_1(A) = \int\limits_{|\psi\rangle \in A} \mathcal{D}|\psi\rangle \; \rho\left(|\psi\rangle\right). \tag{A.19}$$

Here, the symbol $\int \mathcal{D}$ represents functional integration and ρ denotes a functional on $\mathcal{H}$. For bosons and for an arbitrary Schauder basis $\{|\nu\rangle\}$ of $\mathcal{H}$, the functional integration is defined by

$$\int\limits_{\Omega} \mathcal{D}|\psi\rangle \cdots (|\psi\rangle) \equiv \lim_{n\to\infty} \int\limits_{\mathbb{R}} d\Im(c_1) \int\limits_{\mathbb{R}} d\Re(c_1) \cdots \int\limits_{\mathbb{R}} d\Im(c_n) \int\limits_{\mathbb{R}} d\Re(c_n) \quad \cdots \left(\sum_{\nu=1}^{n} c_\nu |\nu\rangle \right) \tag{A.20}$$

Expressing (A.19) verbally, the probability $\mathbb{P}_1(A)$, that the system occupies any state $|\psi\rangle$ in the set A of states, is given by a generalized integral over A weighted with the density functional ρ.

Measurement on fixed state Assume for the system to be in an arbitrary fixed state $|\psi\rangle \in \mathcal{H}$. In quantum physics, performing a measurement on the system usually alters this state. More precisely, it is postulated, that upon measurement the state is randomly transmuted into any element $|\nu\rangle$ of an orthonormal Schauder basis $h = \{|\nu\rangle\}_{\nu\in\mathbb{N}}$ of $\mathcal{H}$. The Schauder basis depends on the measurement scheme and the transition probabilities are given by $\frac{|\langle\nu|\psi\rangle|^2}{\langle\psi|\psi\rangle}$, (where $\langle \bullet \mid \bullet \rangle$ denotes the scalar product of $\mathcal{H}$). Then, the natural statistical model for the uncertainty of the measurements impact on the state of the system is a probability space with sample space h, where the probability measure is of the form

$$\mathbb{P}_2\left(\{|\nu\rangle\}\right) = \frac{|\langle \nu \mid \psi \rangle|^2}{\langle \psi \mid \psi \rangle}. \tag{A.21}$$

Measurement on unperturbed system The uncertainty of the state of the system prior to the measurement and after the measurement are now merged into a single probability space. In order to take into account all imaginable transitions from any state in $\mathcal{H}$ to any state in h, one assumes a measureable space with sample space $\mathcal{H} \times \{|\nu\rangle\}_{\nu \in \mathbb{N}}$. It is then equipped with a probability measure $\mathbb{P}$ that reduces to $\mathbb{P}_1$ or $\mathbb{P}_2$ under the appropiate circumstances. The probability $\mathbb{P}_1(A)$ of the system starting out in any state in A – irrespective of what state it transitions into – ought to be given by

$$\mathbb{P}_1(A) = \mathbb{P}(A \times h), \tag{A.22}$$

while the probability $\mathbb{P}_2(A')$ of transitioning to any state in A' under the condition of starting out in the state $|\psi\rangle$ ought to be expressible as the limit

$$\mathbb{P}_2(A') = \lim_{A \searrow \{|\psi\rangle\}} \frac{\mathbb{P}(A \times A')}{\mathbb{P}(A \times h)} \tag{A.23}$$

of conditional probabilities. A probability measure $\mathbb{P}$ with these proberties is given by

$$\mathbb{P}(A \times A') \equiv \sum_{|\nu\rangle \in A'} \int_{|\psi\rangle \in A} \mathcal{D}|\psi\rangle \; \rho\left(|\psi\rangle\right) \frac{|\langle \nu \mid \psi \rangle|^2}{\langle \psi \mid \psi \rangle}, \tag{A.24}$$

where both $A \subset \mathcal{H}$ and $A' \subset h$ are measurable sets. Here, $\mathbb{P}(A \times A')$ is to be interpreted as the probability of the unperturbed system starting in any state in A and transitioning to any state in A' upon measurement.

In the microscopic quantum-mechanical description, any physical quantity corresponds to an operator $\hat{X}$ on $\mathcal{H}$. In the new statistical framework, the measurement of such a quantity is interpreted as a random variable $\tilde{X}$. More precisely, it is postulated, that the corresponding random variables are of the shape

$$\tilde{X}\left(|\psi\rangle, |\nu\rangle\right) \equiv \frac{\left\langle \nu \middle| \hat{X} \middle| \psi \right\rangle}{\langle \nu | \psi \rangle}. \tag{A.25}$$

For random variables of this form, the expectation value may be expressed as

$$\mathbb{E}\left(\tilde{X}\right) = \sum_{|\nu\rangle \in h} \int_{|\psi\rangle \in \mathcal{H}} \mathcal{D}|\psi\rangle \; \tilde{X}\left(|\psi\rangle, |\nu\rangle\right) \rho\left(|\psi\rangle\right) \frac{|\langle \nu \mid \psi \rangle|^2}{\langle \psi \mid \psi \rangle} = \sum_{|\nu\rangle \in h} \left\langle \nu \middle| \hat{X}\hat{\rho} \middle| \nu \right\rangle = \mathrm{Tr}\left(\hat{X}\hat{\rho}\right) \tag{A.26}$$

where the so-called density operator

$$\hat{\rho} \equiv \int_{|\psi\rangle \in \mathcal{H}} \mathcal{D}|\psi\rangle \; \rho\left(|\psi\rangle\right) \frac{|\psi\rangle\langle\psi|}{\langle \psi \mid \psi \rangle} \tag{A.27}$$

is identified. The density operator is evidently selfadjoint and inherits $\mathrm{Tr}\left(\hat{\rho}\right) = 1$ from the density functional with $\int_{|\psi\rangle \in \mathcal{H}} \mathcal{D}|\psi\rangle \; \rho = 1$.

B Functional derivative

The functional derivative is a concept from infinite dimensional analysis that constitutes a generalization of the gradient.

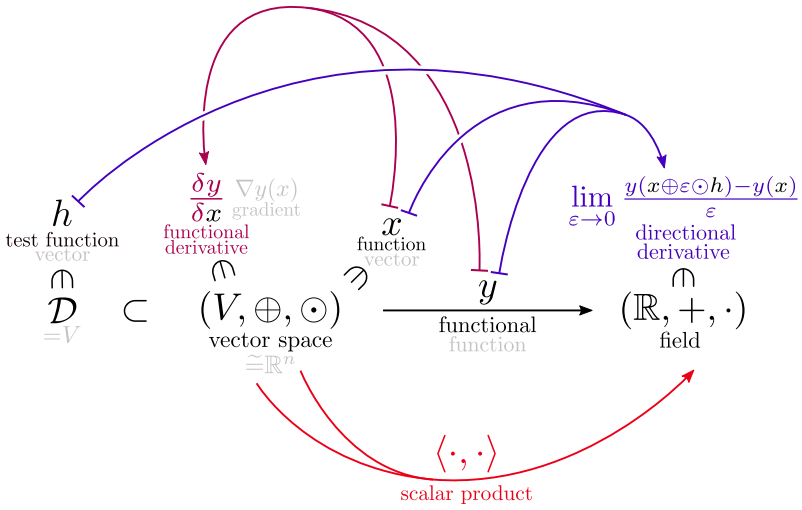
In finite dimensional analysis, for a function $y \in C^2(E, \mathbb{R})$ (with $E \subset \mathbb{R}^n$ open and $n \in \mathbb{N}$) to have a local maximum in $x \in E$, the directional derivative of y at the point x in any direction $h \in \mathbb{R}^n$ has to be zero. Additional sufficient conditions – like the Hesse matrix of y being negative definite at the point x – are not considered here. Applying the chainrule, the necessary condition can be rewritten as

$$0 = \lim_{\varepsilon \to 0} \frac{y(x+\varepsilon h) - y(x)}{\varepsilon \sqrt{\langle h, h \rangle_{\text{euc}}}} = \frac{1}{\sqrt{\langle h, h \rangle_{\text{euc}}}} \frac{dy \circ (x + \bullet h)}{d\varepsilon}(0) = \frac{dy}{dx}(x) \frac{h}{\sqrt{\langle h, h \rangle_{\text{euc}}}} = \left\langle \nabla y(x), \frac{h}{\sqrt{\langle h, h \rangle_{\text{euc}}}} \right\rangle_{\text{euc}}, \tag{B.1}$$

where $\langle \cdot, \cdot \rangle_{\text{euc}}$ denotes the euclidean scalar product. This is obviously equivalent to $\nabla y(x) = 0$, where the gradient is uniquely defined by

$$\forall h \in \mathbb{R}^n : \quad \lim_{\varepsilon \to 0} \frac{y(x+\varepsilon h) - y(x)}{\varepsilon} = \langle \nabla y(x), h \rangle_{\text{euc}} ; \tag{B.2}$$

phrased in words: The gradient of the function y evaluated at the vector x is defined as the vector $\nabla y(x)$, such that the directional derivative of y in any direction $h \in \mathbb{R}^n$ is given by the euclidean scalar product of $\nabla y(x)$ and h. The functional derivative is defined in complete analogy: Let V be a vectorspace. The functional derivative of a functional $y \in V$ evaluated at the function x is defined as the function $\frac{\delta y}{\delta x}$, such that the directional derivative of y in any direction $h \in \mathcal{D} \subset V$ is given by the scalarproduct $\langle \frac{\delta y}{\delta x}, h \rangle$, if it exists. A condensed explanation of the concept of the functional derivative as an abstraction of the gradient is depicted in figure 5. Here $\mathcal{D}$ denotes some dense subset of V, the elements of which are commonly refered to as test functions.



$$\left\langle \frac{\delta y}{\delta x}, h \right\rangle = \lim_{\varepsilon \to 0} \frac{y(x \oplus \varepsilon \odot h) - y(x)}{\varepsilon}$$

Figure 5: Diagram showing the interconnections between the algebraic structures involved in the concept of the functional derivative. The emphasis lies on the definition of the functional derivative from the interplay of the directional derivative and the scalar product. In addition to the general case the particular notation and nomenclature for finite dimensional analysis is provided in light grey.

Under certain assumptions, the functional derivative exhibits some form of the fundamental differentiation rules from finite dimensional analysis (e.g. factor, summation, product and chain rule), which can be derived using the limit theorems.

A special setup relevant to ensemble theory is onsidered. Let V be a space of functions mapping from any set to $\mathbb{R}$. Further, let y be a functional of the form $y(x) = \langle c \circ x, x\rangle$ with $c \in C^1(\mathbb{R}, \mathbb{R})$ and let the linear operator of pointwise multiplication with any element from V be selfadjoint. Then it holds for any test function $h \in \mathcal{D}$

$$\begin{aligned}
\left\langle \frac{\delta y}{\delta x}, h \right\rangle &= \lim_{\varepsilon\to 0} \frac{y(x \oplus \varepsilon \odot h) - y(x)}{\varepsilon} \\
&= \lim_{\varepsilon\to 0} \frac{\langle c \circ (x \oplus \varepsilon \odot h), x \oplus \varepsilon \odot h\rangle - \langle c \circ x, x\rangle}{\varepsilon} \\
&= \lim_{\varepsilon\to 0} \langle c \circ (x \oplus \varepsilon \odot h), h\rangle + \underbrace{\left\langle \frac{c \circ (x \oplus \varepsilon \odot h) - c \circ x}{\varepsilon}, x \right\rangle}_{=\left\langle \frac{dc}{dz} \circ xh, x\right\rangle = \left\langle x, \frac{dc}{dz} \circ xh\right\rangle = \left\langle x \frac{dc}{dz} \circ x, h\right\rangle} \\
&= \left\langle c \circ x + x \frac{dc}{dz} \circ x, h \right\rangle \\
&= \left\langle \frac{d \bullet c(\bullet)}{dz} \circ x, h \right\rangle . \qquad \text{(B.3)}
\end{aligned}$$

Consequently the functional derivative is identified as

$$\frac{\delta y}{\delta x} = \frac{d \bullet c(\bullet)}{dz} \circ x. \qquad \text{(B.4)}$$

C Differential geometry

The main concepts of finite dimensional analysis are generalized. The commonly known definitions of integration and differentiation are only applicable to functions defined on open sets in $\mathbb{R}^n$. By postulating abstract relaxations of the defining properties of the integral and of some differential operators, their domain is greatly expanded.

Let M be a smooth m-dimensional submanifold of $\mathbb{R}^n$. To keep the notation simple, it is assumed that the manifold can be parametrized by a single map φ with codomain $U \subseteq \mathbb{R}^m$ open

$$\begin{array}{rccc} \varphi: & U & \to & M \\ & y & \mapsto & \varphi(y). \end{array} \tag{C.1}$$

C.1 Integration on manifolds

For a function $f : M \to \mathbb{R}$ with $f \circ \varphi \in C^\infty(U, \mathbb{R})$ its integral over M is defined as the Riemann integral of the composition $f \circ \varphi$ weighted with some kind of generalized volume element over U, i.e.

$$\int_M f(x)\, dx \equiv \int_U f(\varphi(y)) \sqrt{\left|\det\left(g(y)\right)\right|}\, dy \tag{C.2}$$

where the metric tensor

$$g(y) \equiv \frac{d\varphi}{dy}^\top(y) \frac{d\varphi}{dy}(y) \tag{C.3}$$

is introduced. The defining property of expression (C.2) is its' invariance under reparametrization. For two maps $\varphi : E \to M$ and $\varphi' : E' \to M$ (with $E' \subset \mathbb{R}^m$ open) the function $\Phi \equiv \varphi^{-1} \circ \varphi' \in C^\infty(E', E)$ is defined. Then, it holds

$$\begin{aligned} &\det\left(g'(y)\right) \\ =&\det\left(\frac{d\varphi'}{dy}(y) \frac{d\varphi'}{dy}^\top(y)\right) \\ =&\det\left(\frac{d\varphi \circ \Phi}{dy}^\top(y) \frac{d\varphi \circ \Phi}{dy}(y)\right) \\ =&\det\left(\frac{d\Phi}{dy}^\top(y) \frac{d\varphi}{dy}^\top\left(\Phi(y)\right) \frac{d\varphi}{dy}\left(\Phi(y)\right) \frac{d\Phi}{dy}(y)\right) \\ =&\det\left(\frac{d\varphi}{dy}^\top\left(\Phi(y)\right) \frac{d\varphi}{dy}\left(\Phi(y)\right)\right) \det\left(\frac{d\Phi}{dy}(y)\right)^2 \\ =&\det\left(g\left(\Phi(y)\right)\right) \det\left(\frac{d\Phi}{dy}(y)\right)^2 \end{aligned} \tag{C.4}$$

$$\begin{aligned} &\int_{U'} f \circ \varphi'(y) \sqrt{\left|\det\left(g'(y)\right)\right|}\, dy \\ =&\int_{U'} f \circ \varphi\left(\Phi(y)\right) \sqrt{\left|\det\left(g\left(\Phi(y)\right)\right)\right|} \left|\det\left(\frac{d\Phi}{dy}\right)\right|\, dy \\ =&\int_{U=\Phi(U')} f \circ \varphi(y') \sqrt{\left|\det\left(g(y')\right)\right|}\, dy'. \end{aligned} \tag{C.5}$$

The integral formula (C.2) is a very versatile tool. For example, it encompasses the usual expressions for path, surface and volume integrals for $n = 3$; as for $m = 1$, $m = 2$ and $m = 3$ the generalized volume element can be rearranged into the common line element, surface element and volume element, respectively:

$m = 1$:

$$\frac{d\varphi}{dy}^\top \frac{d\varphi}{dy} = \left\| \frac{d\varphi}{dy} \right\|^2 \Rightarrow \sqrt{\left| \det \left(\frac{d\varphi}{dy}^\top \frac{d\varphi}{dy} \right) \right|} = \left\| \frac{d\varphi}{dy} \right\| \tag{C.6}$$

$m = 2$:

$$\begin{aligned} \frac{d\varphi}{dy}^\top \frac{d\varphi}{dy} &= \begin{pmatrix} \frac{d\varphi}{dy_1}^\top \\ \frac{d\varphi}{dy_2}^\top \end{pmatrix} \begin{pmatrix} \frac{d\varphi}{dy_1} & \frac{d\varphi}{dy_2} \end{pmatrix} = \begin{pmatrix} \frac{d\varphi}{dy_1} \cdot \frac{d\varphi}{dy_1} & \frac{d\varphi}{dy_1} \cdot \frac{d\varphi}{dy_2} \\ \frac{d\varphi}{dy_2} \cdot \frac{d\varphi}{dy_1} & \frac{d\varphi}{dy_2} \cdot \frac{d\varphi}{dy_2} \end{pmatrix} \\ \Rightarrow \det \left(\frac{d\varphi}{dy}^\top \frac{d\varphi}{dy} \right) &= \left\| \frac{d\varphi}{dy_1} \right\|^2 \left\| \frac{d\varphi}{dy_2} \right\|^2 \left(1 - \cos \left(\angle \frac{d\varphi}{dy_1}, \frac{d\varphi}{dy_2} \right)^2 \right) = \left\| \frac{d\varphi}{dy_1} \times \frac{d\varphi}{dy_2} \right\|^2 \\ \Rightarrow \sqrt{\left| \det \left(\frac{d\varphi}{dy}^\top \frac{d\varphi}{dy} \right) \right|} &= \left\| \frac{d\varphi}{dy_1} \times \frac{d\varphi}{dy_2} \right\| \end{aligned} \tag{C.7}$$

$m = 3$:

$$\det \left(\frac{d\varphi}{dy}^\top \frac{d\varphi}{dy} \right) = \det \left(\frac{d\varphi}{dy} \right)^2 \Rightarrow \sqrt{\left| \det \left(\frac{d\varphi}{dy}^\top \frac{d\varphi}{dy} \right) \right|} = \left| \det \left(\frac{d\varphi}{dy} \right) \right| \tag{C.8}$$

C.2 Differential operators

Gradient The gradient of smooth functions $f : M \to \mathbb{R}$ defined on the arbitrary smooth manifold M is constructed as an extension of the usual gradient of differentiable functions defined on open subsets of the embedding space $\mathbb{R}^n$. Consider a fixed yet arbitrary point $m \in M$. Let γ be a smooth path in M parametrized as

$$\begin{aligned} \gamma : \ ]-1, 1[&\to M \\ t &\mapsto \gamma(t), \end{aligned} \tag{C.9}$$

with

$$m \equiv \gamma(0). \tag{C.10}$$

The first order taylor polynomial of γ in 0 is given by $\gamma(0) + \bullet \frac{d\gamma}{dt}(0)$ and represents a tangent to the manifold M in m. The vectors $\frac{d\gamma}{dt}(0)$ one gets for any such curve form a subspace of $\mathbb{R}^n$, aptly named the tangent space of M in m and denoted by $T_M(m)$. If M is an open set, then for any $h \in \mathbb{R}^n$ the straight path $\gamma(t) = m + th$ (with $|t|$ sufficiently small) is a smooth path in M and consequently the tangent space coincides with the embedding space. With the help of the path γ the directional derivative of f in m in the direction $h \equiv \frac{d\gamma}{dt}(0)$ is defined as $\frac{df \circ \gamma}{dt}(0)$. The directional derivative is well defined as it turns out to be equal for any two smooth paths that coincide in their first order taylor polynomial. Once again, for M open and using the straight paths one retrieves the common definition of the directional derivative of differentiable functions on M. These intuitive extensions of the notion of the tangent space and of the directional derivative are now combined to define the generalized gradient. The generalized gradient of the function f in m is defined as the vector $\nabla f(m) \in T_M(m)$ such that all directional derivatives of f in arbitrary directions $h \in T_M(m)$ can be expressed as the euclidean scalar product of the gradient $\nabla f(m)$ and the direction h, i.e.

$$\nabla f(m) \cdot h = \frac{df \circ \gamma}{dt}(0). \tag{C.11}$$

It turns out to be sufficient to regard only the paths γ of the form $\gamma = \varphi \circ (y_0 + \bullet\eta)$ with $\varphi(y_0) = m$ and arbitrary $\eta \in \mathbb{R}^m$, that can be expressed as a composition of the map φ and a straight path in U. These paths do already exhaust all possible directions in the tangent space, which turns out to be given

by the column space of $\frac{d\varphi}{dy}(y_0)$. The set of linear equations for $\nabla f(m)$ resulting from this set of paths reads

$$\nabla f(m)^\top \frac{d\varphi}{dy}(y_0) = \frac{df \circ \varphi}{dy}(y_0). \tag{C.12}$$

Additionally, since the gradient is defined as an element of the tangent space $T_M(m)$, it can be written as a linear combination of the columns of $\frac{d\varphi}{dy}(y_0)$ with the coefficients comprised in a vector $\lambda \in \mathbb{R}^m$, i.e. $\nabla f(m) = \frac{d\varphi}{dy}(y_0)\lambda$. Inserting this linear combination into the system of linear equations yields λ:

$$\begin{aligned} \lambda^\top \frac{d\varphi}{dy}^\top (y_0) \frac{d\varphi}{dy}(y_0) &= \frac{df \circ \varphi}{dy}(y_0) \\ \Leftrightarrow \lambda &= g^{-1}(y_0) \frac{df \circ \varphi}{dy}(y_0)^\top. \end{aligned} \tag{C.13}$$

Finally, the generalized gradient reads

$$\nabla f(m) = \frac{d\varphi}{dy}(y_0) g^{-1}(y_0) \frac{df \circ \varphi}{dy}^\top (y_0). \tag{C.14}$$

As expected, if the manifold M is an open set in $\mathbb{R}^n$ and the map φ is the identity, then one retrieves the usual expression $\nabla f(y_0) = \frac{df}{dy}^\top (y_0)$. In retrospect, it is also verified that the generalized gradient is well defined in the sense that it doesen't depend on choice of the map φ. For a second map $\varphi' : E' \to M$ with $E' \subset \mathbb{R}^m$ open and $\phi \equiv \varphi'^{-1} \circ \varphi \in C^\infty(U, U')$, the metric tensor is expressed as

$$\begin{aligned} g\left(\varphi(y)\right) &= \frac{d\varphi}{dy}^\top (y) \frac{d\varphi}{dy}(y) \\ &= \frac{d\varphi' \circ \phi}{dy}^\top (y) \frac{d\varphi' \circ \phi}{dy}(y) \\ &= \frac{d\phi}{dy}^\top (y) \frac{d\varphi'}{dy}^\top \left(\phi(y)\right) \frac{d\varphi'}{dy}\left(\phi(y)\right) \frac{d\phi}{dy}(y) \\ &= \frac{d\phi}{dy}^\top (y) g'\left(\varphi'\left(\phi(y)\right)\right) \frac{d\phi}{dy}(y). \end{aligned} \tag{C.15}$$

By using this result in the calculation

$$\begin{aligned} \nabla f\left(\varphi(y)\right) &= \frac{d\varphi}{dy}(y) g^{-1}\left(\varphi(y)\right) \frac{df \circ \varphi}{dy}^\top (y) \\ &= \frac{d\varphi' \circ \phi}{dy}(y) g^{-1}\left(\varphi(y)\right) \frac{df \circ \varphi' \circ \phi}{dy}^\top (y) \\ &= \frac{d\varphi'}{dy}\left(\phi(y)\right) \frac{d\phi}{dy}(y) g^{-1}\left(\varphi(y)\right) \frac{d\phi}{dy}^\top (y) \frac{df \circ \varphi'}{dy}^\top \left(\phi(y)\right) \\ &= \frac{d\varphi'}{dy}\left(\phi(y)\right) g'^{-1}\left(\varphi'\left(\phi(y)\right)\right) \frac{df \circ \varphi'}{dy}^\top \left(\phi(y)\right) \\ &= \nabla f\left(\varphi' \circ \phi(y)\right), \end{aligned} \tag{C.16}$$

it becomes apparent that the gradient is indeed invariant under reparametrization.

Divergence A smooth vector field F on the manifold M is defined as a function mapping each point $m \in M$ to a vector in the local tangent space $T_M(m)$

$$\begin{aligned} F:\ & M \to \mathbb{R}^n \\ & m \mapsto F(m) \in T_M(m) \end{aligned} \tag{C.17}$$

with $F \circ \varphi \in C^\infty(U, \mathbb{R}^n)$. It can be alternatively expressed as $F \circ \varphi(y) = \frac{d\varphi}{dy}(y)\tilde{F}(y)$ with a function $\tilde{F} \in C^\infty(U, \mathbb{R}^m)$. Its generalized divergence is constructed as an extension of the usual divergence for differentiable functions defined on open sets. To this end the previous extensions of the notion of integration and of the gradient are combined. The divergence of F is defined as the smooth function $\nabla \cdot F : M \to \mathbb{R}$, such that for any smooth function $f : M \to \mathbb{R}$ with $f \circ \varphi \in C_c^\infty(U, \mathbb{R})$ it holds

$$\int_M f(m) \nabla \cdot F(m)\ dm = -\int_M \nabla f(m) \cdot F(m)\ dm. \tag{C.18}$$

Here the symbol $\cdot$ to the right of the equality denotes the euclidean scalar product on $\mathbb{R}^n$. This postulate is an extension of the usual integration by parts with the boundary terms equal to zero. Inserting the definitions of the integral and of the gradient one gets

$$\begin{aligned}
&\int_U f\left(\varphi(y)\right) \nabla \cdot F\left(\varphi(y)\right) \sqrt{\left|\det\left(g(y)\right)\right|}\ dy \\
&= -\int_U \frac{df \circ \varphi}{dy}(y) g^{-1}(y) \frac{d\varphi}{dy}^\top (y) F \circ \varphi(y) \sqrt{\left|\det\left(g(y)\right)\right|}\ dy \\
&= -\int_U \frac{df \circ \varphi}{dy}(y) \tilde{F}(y) \sqrt{\left|\det\left(g(y)\right)\right|}\ dy \\
&= \int_U f \circ \varphi(y) \sum_{i=1}^m \frac{d}{dy_i} \left(\tilde{F}_i(y) \sqrt{\left|\det\left(g(y)\right)\right|} \right)\ dy.
\end{aligned} \tag{C.19}$$

In the last equality, the usual integration by parts was performed, where the compact support of $f \circ \varphi$ ensures that no boundary terms arise. Due to the arbitrariness of f one can identify the generalized divergence of F in $\varphi(y)$ as

$$\nabla \cdot F\left(\varphi(y)\right) = \frac{1}{\sqrt{\left|\det\left(g(y)\right)\right|}} \sum_{i=1}^m \frac{d}{dy_i} \left(\tilde{F}_i(y) \sqrt{\left|\det\left(g(y)\right)\right|} \right). \tag{C.20}$$

It remains to remark that the generalized divergence is well defined, since its definintion includes only the generalized gradient and the generalized integral, both of which are invariant under reparametrization.

Laplace-Beltrami All previous generalizations culminate in the definition of the Laplace-Beltrami operator Δ. The result of the Laplace-Betrami operator acting on a smooth function f on the manifold M is defined as the smooth function

$$\Delta f \equiv \nabla \cdot \nabla f, \tag{C.21}$$

that is, the divergence of the vectorfield $F \equiv \nabla f$ given by the gradient of f. This obviously constitutes a generalization of the usual Laplace operator which acts only on functions defined on open sets. From $F\left(\varphi(y)\right) = \nabla f\left(\varphi(y)\right) = \frac{d\varphi}{dy}(y) g^{-1}(y) \frac{df \circ \varphi}{dy}(y)$ one reads off, that $\tilde{F}(y) = g^{-1}(y) \frac{df \circ \varphi}{dy}(y)$. Inserting this into the definition of the Laplace-Beltrami operator directly yields

$$\Delta f\left(\varphi(y)\right) = \frac{1}{\sqrt{\left|\det\left(g(y)\right)\right|}} \sum_{i=1}^m \frac{d}{dy_i} \left(\sqrt{\left|\det\left(g(y)\right)\right|} g^{-1}_{i\bullet}(y) \frac{df \circ \varphi}{dy}(y) \right). \tag{C.22}$$

The notation $g^{-1}_{i\bullet}(y)$ denotes the i-th row of the inverse of the matrix $g(y)$. The well-definedness of the Laplace-Beltrami operator is inherited from its constituents, namely the generalized gradient and the genralized divergence. From the definitions (C.18) of the generalized divergence and (C.21) of the Laplace-Beltrami operator follows the consideration

$$\int_M f \Delta f\ dx = -\int_M \nabla f \cdot \nabla f\ dx \leq 0, \tag{C.23}$$

which entails the important property, that the eigenvalues of the Laplace-Beltrami operator are real and nonpositive.

C.3 Example

To give an example, the specific case $n = 3$, $m = 2$ with the manifold $M = \partial B_r(0) \subset \mathbb{R}^3$ is considered. The manifold M can be parametrized by the map

$$\begin{aligned} \varphi : \ ]0, 2\pi[\times]0, \pi[&\to \partial B_r(0) \\ \vartheta_1, \vartheta_2 &\mapsto r \begin{pmatrix} \cos(\vartheta_1)\sin(\vartheta_2) \\ \sin(\vartheta_1)\sin(\vartheta_2) \\ \cos(\vartheta_2) \end{pmatrix}. \end{aligned} \tag{C.24}$$

(From a technical standpoint, a second map would be needed to provide open coverage of the points on the line $\varphi(0, \bullet)$, where openness is meant with respect to the subspace topology of M embedded in $\mathbb{R}^3$, but may be omitted here). The Jacobimatrix of φ reads

$$\frac{d\varphi}{d(\vartheta_1, \vartheta_2)} = r \begin{pmatrix} -\sin(\vartheta_1)\sin(\vartheta_2) & \cos(\vartheta_1)\cos(\vartheta_2) \\ \cos(\vartheta_1)\sin(\vartheta_2) & \sin(\vartheta_1)\cos(\vartheta_2) \\ 0 & -\sin(\vartheta_2) \end{pmatrix} \tag{C.25}$$

and consequently the metric tensor evaluates to

$$g(\vartheta_1, \vartheta_2) = \begin{pmatrix} r^2 \sin(\vartheta_2)^2 & 0 \\ 0 & r^2 \end{pmatrix} \tag{C.26}$$

The integration of a smooth function f over M then takes the well known shape

$$\int_M f(m)\ dm = \int_0^{2\pi} d\vartheta_1 \int_0^{\pi} f \circ \phi(\vartheta_1, \vartheta_2) r^2 \sin(\vartheta_2)\ d\vartheta_2\ d\vartheta_1. \tag{C.27}$$

Likewise, the Laplace-Beltrami operator simplifies to the well known result

$$\begin{aligned} \Delta f\left(\varphi(y)\right) &= \frac{1}{r^2 \sin(\vartheta_2)} \sum_{i=1}^{2} \frac{d}{d\vartheta_i} \left(r^2 \sin(\vartheta_2) \begin{pmatrix} r^{-2}\sin(\vartheta_2)^{-2} & 0 \\ 0 & r^{-2} \end{pmatrix}_{i\bullet} \frac{df \circ \varphi}{d(\vartheta_1, \vartheta_2)}(y) \right) \\ &= \frac{1}{r^2} \left(\frac{1}{\sin\vartheta_2} \frac{d^2}{d\vartheta_1^2} + \frac{1}{\sin(\vartheta_2)} \frac{d}{d\vartheta_2} \sin(\vartheta_2) \frac{d}{d\vartheta_2} \right) f \circ \varphi(\vartheta_1, \vartheta_2). \end{aligned} \tag{C.28}$$

These results also showcases nicely, how the differentiation and integration of functions on manifolds are traced back to "ordinary" differentiation and integration.

D Scattering theory

The idea of scattering theory is to extract physically meaningful information about an interactive system, by regarding the smallest possible sub-system that still exhibts interaction. In this chapter, second-quantized Schrödinger field theory for free particles with pairwise interaction is considered, the theroretical framework of which is already layed out in chapter 2.1. Here, "free particles" means, that the domain M of the ladder operators $\hat{a}_x$ is given by an entire subspace $M = \mathbb{R}^n$ of $\mathbb{R}^3$. As the interaction is pairwise, the smallest subsystem with interaction is the two-particle system, which is investigated in detail in this appendix.

To any state $|\psi(\bullet)\rangle$ of the second-quantized description a corresponding two-particle state φ is assigned via a projection onto the states $\hat{a}^\dagger_{x_1}\hat{a}^\dagger_{x_2}|0\rangle$ like

$$\varphi(x_1, x_2, t) \equiv \langle 0 \mid \hat{a}_{x_1}\hat{a}_{x_2} \mid \psi(t)\rangle. \tag{D.1}$$

Since $\hat{a}_{x_1}$ and $\hat{a}_{x_2}$ commute, for φ to be well defined, it has to be symmetric under permutation of the arguments x_1 and x_2. However, as this condition plays a negligible role for the following considertions, it is henceforth neglected. From the second quantized Schrödinger equation (2.1) then follows the time-dependent two-particle Schrödinger equation

$$\left(-\frac{\hbar^2}{2m}\Delta_{x_1} - \frac{\hbar^2}{2m}\Delta_{x_2} + V(x_1 - x_2)\right)\varphi\left(x_1, x_2, t\right) = i\hbar\frac{d}{dt}\varphi\left(x_1, x_2, t\right). \tag{D.2}$$

This equation of motion is partially solved and interpreted in the remainder of this appendix.

D.1 Green's function of the Helmholtz operator

Before treating the Schrödinger equation (D.2) itself, as an auxiliary, the Helmoltz equation is investigated. For any $\kappa \in \mathbb{R}$ the Helmholtz differential operator and its' Green's function $G_\kappa : \mathbb{R}^n \to \mathbb{C}$ are defined by

$$\left(\Delta_x + \kappa^2\right) G_\kappa(x - x') = \delta(x - x'). \tag{D.3}$$

Applying a Fourier transformation to this equation yields

$$(2\pi)^{-\frac{n}{2}} = \mathcal{F}\left(\delta\right)(q) = \mathcal{F}\left((\Delta_x + \kappa^2)G_\kappa(\bullet)\right)(q) = \left(i^2\|q\|^2 + \kappa^2\right)\mathcal{F}\left(G_\kappa(\bullet)\right)(q). \tag{D.4}$$

With a subsequent inverse Fourier transformation, the Green's function is then expressed by the integral

$$G_\kappa(x - x') = \mathcal{F}^{-1}\left(\frac{(2\pi)^{-\frac{n}{2}}}{\kappa^2 - \|\bullet\|^2}\right)(x - x') = (2\pi)^{-n}\int\limits_{\mathbb{R}^n}\frac{e^{iq\cdot(x-x')}}{\kappa^2 - \|q\|^2}\, dq. \tag{D.5}$$

In the following the integral is evaluated for the specific cases $n \in \{2, 3\}$

Three-dimensional case Specializing on $n = 3$, the multi-dimensional integral in (D.5) is reduced to a one-dimensional integral by employing spherical coordinates (with the axis corresponding to $\vartheta = 0$ aligned with $x - x'$):

$$\begin{aligned}
\int_{\mathbb{R}^3} \frac{e^{iq\cdot(x-x')}}{\kappa^2 - \|q\|^2}\, dq &= \int_0^{2\pi} d\varphi \int_0^{\pi} d\vartheta\ \sin(\vartheta) \int_0^{\infty} dq\ q^2\ \frac{e^{iq\|x-x'\|\cos(\vartheta)}}{\kappa^2 - q^2} \\
&= 2\pi \int_0^{\infty} dq\ \frac{q^2}{\kappa^2 - q^2} \underbrace{\int_0^{\pi} d\vartheta\ \sin(\vartheta) e^{iq\|x-x'\|\cos(\vartheta)}}_{= \frac{i}{q\|x-x'\|}\left[e^{iq\|x-x'\|\cos(\vartheta)}\right]_0^{\pi}} \\
&\qquad = \tfrac{i}{q\|x-x'\|}\left(e^{-iq\|x-x'\|} - e^{iq\|x-x'\|}\right) \\
&= -\frac{2\pi i}{\|x-x'\|} \int_0^{\infty} \frac{q}{\kappa^2 - q^2} e^{iq\|x-x'\|} + \frac{-q}{\kappa^2 - (-q)^2} e^{i(-q)\|x-x'\|}\, dq \\
&= \frac{2\pi i}{\|x-x'\|} \int_{\mathbb{R}} \frac{q}{q^2 - \kappa^2} e^{iq\|x-x'\|}\, dq. \qquad \text{(D.6)}
\end{aligned}$$

The remaining integral is solved by applying the residue theorem. Consider a complex contour integral along a half circle $]-Q, Q[\cup\{Qe^{i\alpha} | 0 < \alpha < \pi\}$ of radius $Q \in \mathbb{R}^+$ in counter clockwise direction. The itegral over $\mathbb{R}$ then corresponds to the limit $Q \to \infty$ of this contour integral. The contribution from the arc vanishes since the integrand decays exponentially for $\Im(q) \to \infty$ and decays linearly for $|\Re(q)| \to \infty$. To avoid poles of the integrand on the contour, an imaginary number $-i\eta$ with $\eta \in \mathbb{R}$ is added to the denominator of the integrand. The poles can then be calculated as the zeros of the denominator up to first order in η by quadratic completion:

$$\begin{aligned}
&\kappa^2 + i\eta = \kappa^2 + 2\kappa\frac{i\eta}{2\kappa} + \left(\frac{i\eta}{2\kappa}\right)^2 - \left(\frac{i\eta}{2\kappa}\right)^2 = \left(\kappa + \frac{i\eta}{2\kappa}\right)^2 + \mathcal{O}(\eta^2) \\
\Rightarrow\quad &\frac{1}{q^2 - \kappa^2 - i\eta} = \frac{1}{q^2 - \left(\kappa + \frac{i\eta}{2\kappa}\right)^2 + \mathcal{O}(\eta^2)} = \frac{1}{\left(q - \left(\kappa + \frac{i\eta}{2\kappa}\right)\right)\left(q + \left(\kappa + \frac{i\eta}{2\kappa}\right)\right)} + \mathcal{O}(\eta^2)
\end{aligned}$$

Therewith applying the residue theorem yields

$$\begin{aligned}
&\int_{\mathbb{R}} \frac{q}{q^2 - \kappa^2} e^{iq\|x-x'\|}\, dq \\
&= \lim_{\pm\eta \searrow 0} \int_{\mathbb{R}} \frac{q}{q^2 - \kappa^2 - i\eta} e^{iq\|x-x'\|}\, dq \\
&= 2\pi i \lim_{\pm\eta \searrow 0} \lim_{q \to \pm\kappa \pm \frac{i\eta}{2\kappa}} \frac{q}{q \pm \kappa \pm \frac{i\eta}{2\kappa}} e^{iq\|x-x'\|} \\
&= 2\pi i \lim_{\pm\eta \searrow 0} \frac{1}{2} e^{\pm i\left(\kappa + \frac{i\eta}{2\kappa}\right)\|x-x'\|} \\
&= i\pi\ e^{\pm i\kappa\|x-x'\|} \qquad \text{(D.7)}
\end{aligned}$$

and the limit $\eta \to 0$ is performed afterwards. Caution is due, as this limit is ill-defined and one has to instead differentiate the two cases $\lim_{\eta \searrow 0}$ and $\lim_{\eta \nearrow 0}$. As the Helmholtz operator is of order two, these two cases correspond to its two linearly independent fundamental solutions. Consequently, by inserting (D.6) and (D.7) back into equation (D.5), one gets the two linearly independent canditates

$$G_\kappa(x - x') = -\frac{1}{4\pi} \frac{e^{\pm i\kappa\|x-x'\|}}{\|x-x'\|} \qquad \text{(D.8)}$$

for the Green's function of the Helmholtz differential operator in three dimensions.

Two-dimensional case In the case $n = 2$ the integral in (D.5) is solved analogously to the the three-dimensional case, by employing polar coordinates (with the axis corresponding to $\varphi = 0$ aligned with $x - x'$):

$$\begin{aligned}\int_{\mathbb{R}^2} \frac{e^{iq\cdot(x-x')}}{\kappa^2 - \|q\|^2}\, dx &= \int_0^\infty d\rho\ \rho \int_0^{2\pi} d\varphi\ \frac{e^{i\rho\|x-x'\|\cos(\varphi)}}{\kappa^2-\rho^2} \\ &= \int_0^\infty d\rho\ \frac{\rho}{\kappa^2-\rho^2} \int_0^{2\pi} d\varphi\ e^{i\rho\|x-x'\|\cos(\varphi)}. \end{aligned} \tag{D.9}$$

According to the compendium [18, eq. 8.411.1] the angular integral may be identified with a Bessel function J_0 of first kind and zeroth order evaluated at $\rho\|x - x'\|$, i.e.

$$J_0\left(\rho\|x-x'\|\right) = \int_0^{2\pi} d\varphi\ e^{i\rho\|x-x'\|\cos(\varphi)}. \tag{D.10}$$

The remaining radial integral may in turn be identified with a modified Bessel function K_0 of zeroth order of the imaginary argument $\pm ik\|x - x'\|$. In order to fulfill the requirements of [18, eq. 6.566.2], a positive real part $\eta > 0$ has to be added to k and the limit $\eta \searrow 0$ is taken afterwards, i.e

$$K_0\left(\pm i\kappa\|x-x'\|\right) = \lim_{\eta\searrow 0} \int_0^\infty d\rho\ \frac{\rho}{\rho^2 + (\pm i\kappa+\eta)^2} J_0\left(\rho\|x-x'\|\right). \tag{D.11}$$

Lastly the modified Bessel function may be expressed as a Hankel function (Besselfunction of the third kind) $H_0^{(1)}$ of zeroth order evaluated at $\mp k\|x - x'\|$ according to [18, eq. 8.407.1]

$$K_0\left(\pm i\kappa\|x-x'\|\right) = \frac{i\pi}{2} H_0^{(1)}\left(\mp\kappa\|x-x'\|\right). \tag{D.12}$$

Consecutively inserting the equations (D.9), (D.10), (D.11) and (D.12) back into (D.5), gives the two linearly independent candidates

$$G_\kappa(x-x') = \frac{i}{4} H_0^{(1)}\left(\mp\kappa\|x-x'\|\right) \tag{D.13}$$

for the Green's functions of the Helmholtz differential operator in two dimensions.

D.2 Center of mass frame

With the help of the coordinate transformation

$$\left.\begin{array}{c} X \equiv \frac{x_1+x_2}{2} \\ x \equiv x_1 - x_2 \end{array}\right\} \Leftrightarrow \left\{\begin{array}{l} x_1 = X + \frac{x}{2} \\ x_2 = X - \frac{x}{2} \end{array}\right. , \tag{D.14}$$

the wavefunction φ is expressed in the center of mass frame by the transformed wavefunction

$$\varphi'(x, X, t) \equiv \varphi\left(x_1(x, X), x_2(x, X), t\right). \tag{D.15}$$

Due to the definitions (D.14) and (D.15), one has the auxiliary calculations

$$\begin{aligned} \frac{dx_k}{dx_{ij}} &= (-1)^{i-1}\delta_{jk} \quad \wedge \quad \frac{dX_k}{dx_{ij}} = \frac{1}{2}\delta_{jk} \\ \frac{d}{dx_{ij}}\varphi(x_1, x_2, t) &= \left((-1)^{i-1}\frac{d}{dx_j} + \frac{1}{2}\frac{d}{dX_j}\right)\varphi'\left(x(x_1,x_2), X(x_1,x_2), t\right) \\ \frac{d^2}{dx_{ij}^2}\varphi(x_1, x_2, t) &= \left(\frac{d^2}{dx_j^2} + \frac{1}{4}\frac{d^2}{dX_j^2} + (-1)^{i-1}\frac{d^2}{dx_j dX_j}\right)\varphi''\left(x(x_1,x_2), X(x_1,x_2), t\right) \end{aligned}$$

for all $i \in \{1,2\}$ and $j,k \in \{1 \cdots n\}$. Therewith, inserting the transformed wavefunction φ' into the Schrödinger equation (D.2) yields

$$\left(-\frac{\hbar^2}{4m}\Delta_X - \frac{\hbar^2}{m}\Delta_x + V(x)\right)\varphi'(x,X,t) = i\hbar\frac{d}{dt}\varphi'(x,X,t)\,. \tag{D.16}$$

Hence, the transformation enables the separation of the variables t, x and X via the product Ansatz

$$\varphi'(x,X,t) = \phi(x)\phi'(X)\phi''(t), \tag{D.17}$$

The Ansatz entails differential equations for each of the three multiplicative components of φ'. For the time-dependent component ϕ'' one gets

$$i\hbar\frac{d}{dt}\phi''(t) = E\phi''(t). \tag{D.18}$$

with an unknown energy $E \in \mathbb{R}$. Likewise, the component ϕ' must obey the differential equation

$$-\frac{\hbar^2}{4m}\Delta_X\phi'(X) = E'\phi'(X). \tag{D.19}$$

with an unknown energy $E' \in \mathbb{R}$. Lastly, the component ϕ has to fulfill the equation

$$\left(-\frac{\hbar^2}{m}\Delta_x + V(x)\right)\phi(x) = (E-E')\phi(x). \tag{D.20}$$

Equation (D.20) is construed as an inhomogenous Helmholtz equation with wavenumber $\kappa = \frac{\sqrt{m(E-E')}}{\hbar}$ and inhomogeneity $\frac{m}{\hbar^2}V(\bullet)\phi(\bullet)$. With the Green's function G_κ of the Helmholtz operator, its solutions ϕ are expressed as

$$\phi(x) = \phi_{\text{inc}}(x) + \phi_{\text{sca}}(x), \tag{D.21}$$

where ϕ_{inc} denotes an arbitrary solution of the homogenous Helmholtz equation and ϕ_{sca} denotes the solution

$$\phi_{\text{sca}} \equiv \int_{\mathbb{R}^n} G_\kappa(x-x')\frac{m}{\hbar^2}V(x')\phi(x')\;dx' \tag{D.22}$$

of the inhomogenous Helmholtz equation. In conjunction, Equations (D.21) and (D.22) are known as the Lippmann-Schwinger equation of the scattering theory. The additive contribution ϕ_{sca} is labeled the scattered wave, as it vanishes without interaction. In contrast, the contribution ϕ_{inc} does not depend on the interaction and is hence called the incoming wave.

D.3 Probabilistic interpretation

By multiplying the time-dependent Schrödinger equation in the center of mass frame (D.16) with φ' and subtracting it from its complex conjugate, one gets the continuity equation

$$-\frac{d}{dt}|\varphi'|^2 = 2\nabla_x \cdot \mathcal{J}_x(\varphi') + \frac{1}{2}\nabla_X \cdot \mathcal{J}_X(\varphi'), \tag{D.23}$$

where $\mathcal{J}$ denotes the non-linear differential operator

$$\mathcal{J}(\bullet) = \frac{i\hbar}{2m}\left(\bullet\nabla_x\,\bullet^* - \bullet^*\,\nabla_x\bullet\right). \tag{D.24}$$

Two properties of $\mathcal{J}$, which are useful for calculations, are the product rule

$$\mathcal{J}(\phi_1\phi_2) = |\phi_1|^2\mathcal{J}(\phi_2) + \mathcal{J}(\phi_1)|\phi_2|^2, \tag{D.25}$$

and

$$\phi_1 : \mathbb{R}^n \to \mathbb{R} \quad \Rightarrow \quad \mathcal{J}(\phi_1) = 0 \tag{D.26}$$

for any two differentiable functions $\phi_1, \phi_2 : \mathbb{R}^n \to \mathbb{C}$.

As is common consensus, $|\varphi(x_1, x_2, t)|^2$ is interpreted as the probability density of the two particles being located around x_1 and x_2, respectively, at time t. Consequently, $|\varphi'(x, X, t)|^2$ is interpreted as the probability density of the two particles residing around a constellation with relative coordinate x and center of mass X, respectively. Together with the continuity equation (D.23) and Gauss's theorem from vector calculus, this entails the interpretation of $\mathcal{J}_x(\varphi')$ and $\mathcal{J}_X(\varphi')$ as the probability density current of the two-particle system "flowing" into constellations with different relative coordinate x and different center of mass X, respectively. The probability current density $\mathcal{J}_x(\varphi')$ is associated with scattering, as it describes the movement of the particles away from or towards one another. With the decomposition (D.17) of φ' and the product rule (D.25) for $\mathcal{J}$ one gets

$$\mathcal{J}_x\left(\varphi'(\bullet, X, t)\right)(x) = \mathcal{J}_x(\phi)(x)|\phi'(X)|^2|\phi''(t)|^2. \tag{D.27}$$

Due to the non-linearity of $\mathcal{J}$, one generally has $\mathcal{J}(\phi) \neq \mathcal{J}(\phi_{\text{inc}}) + \mathcal{J}(\phi_{\text{sca}})$. Nevertheless, both probability current densities $\mathcal{J}(\phi_{\text{inc}})$ and $\mathcal{J}(\phi_{\text{sca}})$ are regarded separately, as they qualitatively differ in their physical interpretation.

On the one hand, true scattering only takes into account those trajectories, where the particles move away from one another indefinetly as a consequence of the interaction. Therefore, only the component ϕ_{sca} plays a role. The probability current corresponding to this phenomenon is intuitively given by the surface integral

$$J_{\text{sca}} \equiv \lim_{r\to\infty} \int\limits_{\partial B_r(0)} \mathcal{J}(\phi_{\text{sca}}) \cdot ds. \tag{D.28}$$

On the other hand, the component ϕ_{inc} provides the probability current which can be scattered in the first place. At this stage, one commonly specializes on plane waves for ϕ_{inc}, i.e.

$$\phi_{\text{inc}} \stackrel{!}{=} e^{ik\cdot x}. \tag{D.29}$$

where the wavevector k fulfills $\|k\| = \kappa$. The incoming wave then has a homogenous probability density current

$$\mathcal{J}(\phi_{\text{inc}}) = \frac{\hbar k}{m}. \tag{D.30}$$

The solution ϕ of the Lippmann-Schwinger equation is linear in the incoming wave ϕ_{inc}, as is the scattered wave ϕ_{sca}. The scattered probability current J_{sca} is therefore proportional to $\|\mathcal{J}(\phi_{\text{inc}})\|$, i.e.

$$\sigma(\kappa)\|\mathcal{J}(\phi_{\text{inc}})\| = J_{\text{sca}}, \tag{D.31}$$

where the proportionality constant $\sigma(\kappa)$ is commonly known as the total scattering cross section. The total scattering cross section $\sigma(\kappa)$ is therefore a measure for the total scattering capacity of the interaction potential V for scattering processes characterized by a wavenumber κ. For low energies, or synonymously for low wavenumbers κ, the total cross section is related to a parameter a_s, called the s-wave scattering length, like

$$\sigma(\kappa) + \mathcal{O}(\kappa) = a_s(\kappa)^2 \begin{cases} 4\pi & n = 3 \\ 2\pi & n = 2 \end{cases}. \tag{D.32}$$

D.4 Far field

To evaluate the cross section $\sigma(\kappa)$, an asymptotic expression for the scattered wave at large inter-particle distances $\|x\|$ is needed for equation (D.28). In the integral expression (D.22) for ϕ_{sca}, the Green's function G_κ is consequently evaluated at large $\|x\|$. For $G_\kappa(x-x')$ we have the expressions (D.8) and (D.13) in three and two dimensions, respectively, which only depend on the distance $\|x - x'\|$. This distance is expanded as

$$\begin{aligned}\|x-x'\| &= \sqrt{\|x\|^2 - 2x\cdot x' + \|x'\|^2} \\ &= \|x\|\sqrt{1 - 2\frac{\|x'\|}{\|x\|}\frac{x}{\|x\|}\cdot\frac{x'}{\|x'\|} + \left(\frac{\|x'\|}{\|x\|}\right)^2} \\ &= \|x\|\left(1 - \frac{1}{2}2\frac{\|x'\|}{\|x\|}\frac{x}{\|x\|}\cdot\frac{x'}{\|x'\|} + \mathcal{O}\left(\frac{\|x'\|^2}{\|x\|^2}\right)\right) \\ &= \|x\| - x'\cdot\frac{x}{\|x\|} + \mathcal{O}\left(\frac{\|x'\|}{\|x\|}\right). \end{aligned} \tag{D.33}$$

Since the integration with respect to x' in (D.22) runs over $\mathbb{R}^n$, the fraction $\frac{\|x'\|}{\|x\|}$ is not generally small. The short ranged potential V suppresses the contributions from large $\|x'\|$, though. The far field behaviour of the Green's functions G_κ is derived in the following for two and three dimensions.

Three-dimensional case In the case $n = 3$, the Green's function G_κ is of the form (D.8). Performing the auxiliary calculations

$$e^{i\kappa\|x-x'\|} = e^{i\kappa\|x\|}e^{-i\kappa\frac{x}{\|x\|}\cdot x'}\underbrace{e^{i\kappa\mathcal{O}\left(\frac{\|x'\|}{\|x\|}\right)}}_{=1+\mathcal{O}\left(\frac{\|x'\|}{\|x\|}\right)}$$

$$\frac{1}{\|x-x'\|} = \frac{1}{\|x\|}\frac{1}{1-\mathcal{O}\left(\frac{\|x'\|}{\|x\|}\right)} = \frac{1+\mathcal{O}\left(\frac{\|x'\|}{\|x\|}\right)}{\|x\|}$$

with the help of the far field approximation (D.33), the Green's function is shown to have the asymptotic form

$$G_\kappa(x-x') = -\frac{1}{4\pi}\frac{e^{\pm i\kappa\|x\|}}{\|x\|}e^{\mp i\kappa\frac{x}{\|x\|}\cdot x'} + \mathcal{O}\left(\frac{\|x'\|}{\|x\|}\right). \tag{D.34}$$

Two-dimensional case In two dimensions, the Green's function is given by Equation (D.13). The Hankel function exhibits the asymptotic behaviour

$$H_0^{(1)}(z) = \sqrt{\frac{2}{\pi z}}e^{i\left(z-\frac{\pi}{4}\right)} + \mathcal{O}(z^{-\frac{3}{2}}) \tag{D.35}$$

for $z \in [0,\infty[$ according to [18, eq. 8.451.3]. With this equality and by reusing the auxiliary calculations (D.4), the Green's function turns out to asymptotically behave like

$$G_\kappa(x-x') \approx \frac{1+i}{4\sqrt{\pi\kappa}}\frac{e^{\pm i\kappa\|x\|}}{\sqrt{\|x\|}}e^{\mp i\kappa\frac{x}{\|x\|}\cdot x'} + \mathcal{O}\left(\frac{\|x'\|}{\|x\|}\right). \tag{D.36}$$

In both of the cases $n \in \{2,3\}$, the Green's function decomposes in the far field into a product of spherical wave depending only on the distance $\|x\|$ and a plane wave depending only on the direction $\frac{x}{\|x\|}$. Inserting the asymptotic form (D.34) or (D.36) into (D.22) yields the expression

$$\phi_{\text{sca}}(x) \approx \frac{e^{\pm i\kappa\|x\|}}{\|x\|^{c_n}}C_n\int_{\mathbb{R}^n} e^{\mp i\frac{x}{\|x\|}\cdot x'}V(x')\phi(x')\,dx' \tag{D.37}$$

for the scattered wave, with the exponents $c_2 = \frac{1}{2}$ and $c_3 = 1$ as well as the factors $C_2 = -\frac{1+i}{4\sqrt{\kappa\pi}}\frac{m}{\hbar^2}$ and $C_3 = -\frac{1}{4\pi}\frac{m}{\hbar^2}$, depending on dimensionality n. The multiplicative component

$$\begin{array}{rccc} f: & \partial B_1(0) & \to & \mathbb{C} \\ & \frac{x}{\|x\|} & \mapsto & C_n \int\limits_{\mathbb{R}^n} e^{\mp i \frac{x}{\|x\|}\cdot x'} V(x')\phi(x')\ dx' \end{array} \tag{D.38}$$

of the scattered wave that only depends on the angles $\frac{x}{\|x\|}$, is called the scattering amplitude.

D.5 Total scattering cross section

With the asymptotic form (D.37) of the scattered wave, its probability current density is expressed in the far field as

$$\mathcal{J}(\phi_{\text{sca}}) \approx \mathcal{J}\left(\frac{e^{i\kappa\|\bullet\|}}{\|\bullet\|^{c_n}} f\left(\frac{\bullet}{\|\bullet\|}\right)\right) \tag{D.39}$$

Performing the auxiliary calculations

$$\begin{gathered} \mathcal{J}\left(e^{\pm i\kappa\|\bullet\|}\right) = \pm\frac{\hbar\kappa}{m}\frac{\bullet}{\|\bullet\|} \\ \mathcal{J}\left(\|\bullet\|^{-c_n}\right) = 0 \\ \frac{d}{dx}\frac{x\cdot x'}{\|x\|} = \frac{1}{\|x\|}x' - \frac{x}{\|x\|^3}(x\cdot x') \quad \Rightarrow \quad \mathcal{J}\left(f\left(\frac{\bullet}{\|\bullet\|}\right)\right)(x) \perp x \end{gathered}$$

and applying the product rule for $\mathcal{J}$ again, one gets

$$\mathcal{J}(\phi_{\text{sca}}) \approx \pm\frac{\hbar\kappa}{m}\frac{\bullet}{\|\bullet\|^{2c_n+1}}\left|f\left(\frac{\bullet}{\|\bullet\|}\right)\right|^2 + \mathcal{O}_\perp, \tag{D.40}$$

with $\mathcal{O}_\perp(x) \perp x$. Therewith, performing the integration in (D.28) leads to the expression

$$\begin{aligned} J_{\text{sca}} &= \lim_{r\to\infty} \pm\frac{\hbar\kappa}{m} r^{-2c_n} \int\limits_{\partial B_r(0)} \frac{\bullet}{\|\bullet\|}\left|f\left(\frac{\bullet}{\|\bullet\|}\right)\right|^2 \cdot ds \\ &= \pm\frac{\hbar\kappa}{m}\lim_{r\to\infty} r^{n-1-2c_n} \int\limits_{\partial B_1(0)} |f|^2\ d\Omega \\ &= \pm\frac{\hbar\kappa}{m}\int\limits_{\partial B_1(0)} |f|^2\ d\Omega. \end{aligned} \tag{D.41}$$

for the scattered probability current. Both in two and three dimensions, one has two linearly independent candidates for the Green's function, indicated by the $\pm$ sign in (D.8) and (D.13), respectively. Now, it finally is possible to rule out the candidates that lead to a negative scattered probability current J_{sca} in (D.41), as they physically amount to the particles "being scattered towards" one another, instead of away from each other. From equation (D.31) then finally follows the relation

$$\sigma(\kappa) = \int\limits_{\partial B_1(0)} |f|^2\ d\Omega \tag{D.42}$$

between the the total scattering cross section and the scattering amplitude.

E Avoiding ultraviolet divergencies

In the treatment of the Bose gas in a box, divergent expressions arise, both in the quantum-statistical/ many-particle description as well as in the scattering theory/ two-particle description, which is a common phenomenon in quantum field theory.

E.1 Origin of divergencies

The source of the particular ultraviolet divergencies encountered in section 3 lies in simple-mindedly approximating a general two-particle interaction potential $V : \mathbb{R}^3 \to \mathbb{R}$ by contact interaction $g\delta$, with $g \in \mathbb{R}$ denoting the interaction strength and δ denoting the δ-distribution. It's physically reasonable to choose the parameter g such that V and $g\delta$ have the same s-wave scattering length in the low-energy limit, which is denoted henceforth with the equivalence relation

$$g\delta \sim_{a_s} V. \tag{E.1}$$

A slightly more sophisticated approach lies in approximating V by a scaled Dirac sequence

$$V \approx g_\varepsilon \delta_\varepsilon \tag{E.2}$$

with $\varepsilon \in]0, \infty[$ and $\lim\limits_{\varepsilon \searrow 0} \delta_\varepsilon = \delta$. It is assumed that

$$g_\varepsilon \delta_\varepsilon \sim_{a_s} V \tag{E.3}$$

for all ε and the limit of the interaction strength is denoted by $g \equiv \lim\limits_{\varepsilon \searrow 0} g_\varepsilon$. The new "scaled Dirac sequence" approach only simplifies to the former simple minded "scaled δ-distribution" approach under the assumption that it holds

$$\lim_{\varepsilon \searrow 0} g_\varepsilon \delta_\varepsilon = \left(\lim_{\varepsilon \searrow 0} g_\varepsilon \right) \left(\lim_{\varepsilon \searrow 0} \delta_\varepsilon \right) = g\delta. \tag{E.4}$$

A simple toy model shows a counterexample to this assumption. Assume the scaled Dirac sequence with

$$g_\varepsilon = \sqrt{\varepsilon} \tag{E.5}$$

$$\delta_\varepsilon(x) = \frac{1}{2\epsilon} \begin{cases} 1 & x \in [-\varepsilon, \varepsilon] \\ 0 & \text{else} \end{cases} \tag{E.6}$$

and the expression

$$z \equiv \int_{\mathbb{R}} \frac{1}{\sqrt{|x|}} V(x)\, dx, \tag{E.7}$$

which is envisioned as the analogon to the partition function Z in an actual quantum statistical model. While approximating V with a scaled Dirac sequence leads to the result

$$z \approx \lim_{\varepsilon \searrow 0} \int_{\mathbb{R}} \frac{1}{\sqrt{|x|}} g_\varepsilon \delta_\varepsilon(x)\, dx = \lim_{\varepsilon \searrow 0} \frac{1}{2\sqrt{\varepsilon}} \int_{-\varepsilon}^{\varepsilon} \frac{1}{\sqrt{|x|}}\, dx = \lim_{\varepsilon \searrow 0} 2 = 2, \tag{E.8}$$

approximating V by the scaled $\delta-$ distribution, i.e. applying the invalid limit theorem (E.4) yields the nonsensical expression

$$z \approx \int_{\mathbb{R}} \frac{1}{\sqrt{|x|}} g\delta(x)\, dx = 0\, \infty. \tag{E.9}$$

The analogy to the actual quantum statistical model becomes clearer, when taking the logarithm of z, analogous to the super-canonical potential $\propto \ln(Z)$. Thereby, equation (E.9) is turned into $\ln(z) = \infty - \infty$, which corresponds to the individually divergent quantum fluctuations and mean-field term in the super-canonical potential.

E.2 Regularization

Strangely, the common way of dealing with the divergencies ignores their source and simply tries to redeem the erroneous results. The method is called regularization. In section 3.2.2 a particular regularization scheme, called cutoff regularization, is used to temporarily assign finite values to the divergent expressions. There – seemingly independently in the scattering therory and in the statistical description – an indefinite integral $\int_0^\infty$ is expressed as the limit $\lim_{\Lambda\to\infty}\int_0^\Lambda$ of definite integrals and the limit is dropped. Then, the now regularized/ finite expressions are combined, thereby miraculously cancelling all terms that would diverge in the limit $\lim_{\Lambda\to\infty}$. Taking this limit afterwards consequently produces a finite final result.

E.3 Coarse graining

The cutoff regularization scheme seemingly introduces the parameter Λ "too late", in the sense that the mathematical error has already occured. Inspired by this consideration, a new method is proposed: A set of coarse grained versions of the quantum-mechanical model, dependent on a parameter $\Lambda \in \mathbb{R}$, is regarded right from the beginning. The original system is retrieved in the limit $\lim_{\Lambda\to\infty}$. Now, the approximation of the interaction potential by a scaled Dirac sequence is applied to the coarse grained systems, in the hopes, that the previously invalid limit theroem (E.4) holds for any finite value of Λ. In this case, no divergencies are contracted and in the end, the limit $\lim_{\Lambda\to\infty}$ is performed to retrieve the behaviour of the original system.

Since the scattering theory is an offshoot of the second quantized quantum-mechanical model, the scattering length is also influenced by the coarse graining. Consequently, the scaled Dirac sequence approximation (E.2) is extented to

$$V \approx g_{\varepsilon,\Lambda}\delta_\varepsilon. \tag{E.10}$$

The equivalence relation $\sim_{a_s}$ now also depends on the coarse graining parameter, denoted as $\sim_{a_s}^\Lambda$. For all Λ and all ε, it is then assumed that

$$g_{\varepsilon,\Lambda}\delta_\varepsilon \sim_{a_s}^\Lambda V. \tag{E.11}$$

E.3.1 Coarse graining operator

The fundamental tool for the coarse graining operation is introduced. Consider a vector space of functions mapping from a submanifold $M \subset \mathbb{R}^3$ to $\mathbb{C}$, that comply with a given boundary condition. Assume now, that a Schauder basis of said vector space is given by a set of eigenfunctions ψ_ν of the Laplace-Beltrami operator on M, with corresponding eigenvalues $-\lambda_\nu^2$ and $\lambda_\nu \in [0,\infty[$. The realness and nonpositivity of the eigenvalues are due to (C.23). Further, assume the set to be orthonormal with respect to the scalar product $\langle\bullet,\bullet\rangle \equiv \int_M \bullet^*(x)\,\bullet\,(x)\,dx$, such that any function can be decomposed into

$$\bullet = \sum_\nu \psi_\nu\langle\psi_\nu,\bullet\rangle. \tag{E.12}$$

For functions of this type, the linear endomorphism

$$C_\Lambda(\bullet) = \sum_{\{\nu|\lambda_\nu<\Lambda\}} \psi_\nu\langle\psi_\nu,\bullet\rangle \tag{E.13}$$

is introduced and labeled the coarse graining operator. The operator C_Λ projects a function into the subspace, spanned by the eigenfunctions of the Laplace-Beltrami operator with $\lambda < \Lambda$. It is well defined, as it does not depend on the particular choice of the Schauder basis. Due to the completeness of the functions ψ_ν, the coarse graining operator goes over into the identity as the parameter Λ goes to infinity, i.e.

$$\lim_{\Lambda\to\infty} C_\Lambda = 1. \tag{E.14}$$

For a vector space of functions on $\mathbb{R}^n$, an analogous coarse graining operator is constructed. Instead of a countable Schauder basis, one has to employ the uncountable set of plane waves $\psi_k = (2\pi)^{-\frac{n}{2}} e^{ik\cdot\bullet}$ with $k \in \mathbb{R}^n$. They are eigenfunctions of the Laplace operator with eigenvalue $-\|k\|^2$ and are orthonormal in the sense $\langle \psi_k, \psi_{k'} \rangle = \int_{\mathbb{R}^n} \psi_k^*(x)\psi_{k'}(x)\ dx = \delta(k-k')$. The plane waves form a complete set in the sense that any function is expressible as a continuous superposition

$$\bullet = \int_{\mathbb{R}^n} \psi_k^*(x)\langle \psi_k, \bullet \rangle\ dk = \mathcal{F}^{-1}(\mathcal{F}(\bullet)), \tag{E.15}$$

which is rewritten in the last equality using the Fourier transformation

$$\mathcal{F}(\bullet)(k) = (2\pi)^{-\frac{n}{2}} \int_{\mathbb{R}^n} \bullet(x) e^{-ik\cdot x}\ dx.$$

In this setting, one defines the coarse graining operator as

$$C_\Lambda(\bullet) \equiv \mathcal{F}^{-1}(I_\Lambda \mathcal{F}(\bullet)), \tag{E.16}$$

where

$$I_\Lambda(q) = \begin{cases} 1 & q \in B_\Lambda(0) \\ 0 & \text{else} \end{cases} \tag{E.17}$$

denotes the indicator function on the ball with radius Λ centered around the origin, and $\mathcal{F}$ denotes Fourier transformation. In this case, the effect of the coarse graining opearator is quite intuitive. The operator C_Λ first maps a function to its spectral composition but then only recombines the spatial frequencies below the cutoff Λ, thereby erasing details in the spatial variation of the function. In the limit $\lim_{\Lambda\to\infty}$ the coarse graining operator goes over into the identity.

E.3.2 Application to toy model

To demonstrate the essence of the working mechanism of the proposed method, it is first applied to the already established toy model, in absence of the distracting complexity of an actual quantum statistical model. The coarse graining of the system is executed by applying the coarse graining operator C_Λ in the quantity z like

$$z_\Lambda \equiv \int_{\mathbb{R}} C_\Lambda \left(\frac{1}{\sqrt{|\bullet|}} \right)(x) V(x)\ dx \tag{E.18}$$

and the original model is retrieved through the limit

$$z = \lim_{\Lambda\to\infty} z_\Lambda. \tag{E.19}$$

For any finite value of Λ, the quantity z_Λ is approximated by a scaled Dirac sequence as prescribed by (E.10):

$$z_\Lambda \approx \int_{\mathbb{R}} C_\Lambda \left(\frac{1}{\sqrt{|\bullet|}} \right) g_{\varepsilon,\Lambda}\delta_\varepsilon(x)\ dx. \tag{E.20}$$

For the real quantum-mechanical model, the correct dependence of the interaction strength on Λ arises from the condition (E.11). For the toy model, which doesn't contain an analogon to scattering theory, it is simply postulated:

$$g_{\varepsilon,\Lambda} \equiv \sqrt{\varepsilon} + \sqrt{\frac{\pi}{2\Lambda}}. \tag{E.21}$$

Inserting (E.20) into (E.19) yields the approximation

$$z \approx \lim_{\Lambda\to\infty} \lim_{\varepsilon\searrow 0} \int_{\mathbb{R}} C_\Lambda \left(\frac{1}{\sqrt{|\bullet|}} \right) g_{\varepsilon,\Lambda}\delta_\varepsilon(x)\ dx \tag{E.22}$$

for the quantity z. As an auxiliary to evaluating (E.22), a simpler expression for the coarse grained function $\frac{1}{\sqrt{|\bullet|}}$ is derived. First, its' Fourier transformation is expressed as the integral

$$\mathcal{F}\left(\frac{1}{\sqrt{|\bullet|}}\right)(k) = \frac{1}{\sqrt{2\pi}} \int\limits_{\mathbb{R}} \frac{1}{\sqrt{|x|}} e^{-ikx}\, dx = \sqrt{\frac{2}{\pi}} \int\limits_{0}^{\infty} \frac{1}{\sqrt{x}} cos(|k|x)\, dx = \sqrt{\frac{2}{\pi}} \frac{2}{\sqrt{|k|}} \int\limits_{0}^{\infty} \cos(y^2)\, dy, \quad \text{(E.23)}$$

where the substitution $y = \sqrt{|k|x}$ was employed in the last equality. With the Fourier transformation of $\frac{1}{\sqrt{|\bullet|}}$ being proportional to itself and the imaginary part also vanishing for the inverse Fourier transformation, one has

$$\frac{1}{\sqrt{|\bullet|}} = \mathcal{F}^{-1}\left(\mathcal{F}\left(\frac{1}{\sqrt{|\bullet|}}\right)\right) = \left(\sqrt{\frac{2}{\pi}} \int\limits_{\mathbb{R}} \cos(y^2)\, dy\right)^2 \frac{1}{\sqrt{|\bullet|}}. \quad \text{(E.24)}$$

Thus, the proportionality constant turns out to be 1, where the positive sign can be found with simple geometric considerations. One gets the identity

$$C_\Lambda\left(\frac{1}{\sqrt{|\bullet|}}\right)(x) = \sqrt{\frac{2}{\pi}} \int\limits_{0}^{\Lambda} \frac{1}{\sqrt{k}} cos(kx)\, dk \quad \text{(E.25)}$$

for the coarse grained function $\frac{1}{\sqrt{|\bullet|}}$. Therewith, Equation (E.22) is evaluated, yielding

$$\begin{aligned} z &\approx \lim_{\Lambda\to\infty} \lim_{\varepsilon\searrow 0} \int\limits_{\mathbb{R}} C_\Lambda\left(\frac{1}{\sqrt{|\bullet|}}\right) g_{\varepsilon,\Lambda}\delta_\varepsilon(x)\, dx \\ &= \lim_{\Lambda\to\infty} \left(\lim_{\varepsilon\searrow 0} g_{\varepsilon,\Lambda}\right) \lim_{\varepsilon\searrow 0} \int\limits_{\mathbb{R}} C_\Lambda\left(\frac{1}{\sqrt{|\bullet|}}\right) \delta_\varepsilon(x)\, dx \\ &= \lim_{\Lambda\to\infty} g_{0,\Lambda}\; C_\Lambda\left(\frac{1}{\sqrt{|\bullet|}}\right)(0) \\ &= \lim_{\Lambda\to\infty} \sqrt{\frac{\pi}{2\Lambda}}\, \sqrt{\frac{2}{\pi}} 2\sqrt{\Lambda} = 2, \end{aligned} \quad \text{(E.26)}$$

which is the familiar result from Equation (E.8). Mind, that in the second equality, the limit $\lim\limits_{\varepsilon\searrow 0}$ was applied separately to $g_{\varepsilon\Lambda}$ and to δ_ε, which previously led to the divergent expression (E.9).

E.3.3 Application to Bose gases on manifolds

Now, after sufficient preparation, the coarse graining of the quantum mechanical model introduced in section 2.1 is performed. It is achieved by applying the coarse graining operator (E.13) to the function of ladder operators $\hat{a}_\bullet$, i.e.

$$\hat{a}_x^{(\Lambda)} \equiv C_\Lambda\left(\hat{a}_\bullet\right)(x) = \sum_{\{\kappa|\lambda_\kappa<\Lambda\}} \psi_\kappa(x) \int\limits_M \psi_\kappa^*(x')\hat{a}_{x'}\, dx'. \quad \text{(E.27)}$$

The second quantized Hamilton operator (2.2) is consequently turned into

$$\hat{H}_\Lambda \equiv \int\limits_M \hat{a}_x^{(\Lambda)\dagger} \left(-\frac{\hbar^2}{2m}\Delta\right) \hat{a}_x^{(\Lambda)}\, dx + \frac{1}{2} \int\limits_M \int\limits_M \hat{a}_x^{(\Lambda)\dagger} \hat{a}_{x'}^{(\Lambda)\dagger} V(x-x') \hat{a}_x^{(\Lambda)} \hat{a}_{x'}^{(\Lambda)}\, dx\, dx'. \quad \text{(E.28)}$$

The according I-particle description of the coarse grained system is derived. The I-particle state/wave function ψ is defined pointwise as a projection of the second quantized state $|\Psi(t)\rangle$ onto the Fock states of the coarse grained ladder operators like

$$\psi(x_1, \cdots x_I, t) \equiv \left\langle 0 \middle| \hat{a}_{x_1}^{(\Lambda)} \cdots \hat{a}_{x_I}^{(\Lambda)} \middle| \Psi(t) \right\rangle. \quad \text{(E.29)}$$

From the second quantized Schrödinger equation then follows the I-particle Schrödinger equation

$$i\hbar\frac{d}{dt}\psi(x_1,\cdots x_I,t)=\left\langle 0\middle|\hat{a}_{x_1}^{(\Lambda)}\cdots\hat{a}_{x_I}^{(\Lambda)}\hat{H}_\Lambda\middle|\Psi(t)\right\rangle, \tag{E.30}$$

which is developed further in the following. First, a few auxiliary calculations are performed. The commutation relations

$$\begin{aligned}[\hat{a}_{x_1}^{(\Lambda)},\hat{a}_{x_2}^{(\Lambda)\dagger}]&=\sum_{\{\kappa|\lambda_\kappa<\Lambda\}}\sum_{\{\nu|\lambda_\nu<\Lambda\}}\psi_\kappa(x_1)\psi_\nu^*(x_2)\underbrace{\int_M\int_M\psi_\kappa^*(x_1')\psi_\nu(x_2')[\hat{a}_{x_1'},\hat{a}_{x_2'}^\dagger]\;dx_1'\;dx_2'}_{=\int_M\psi_\kappa^*(x_1')\psi_\nu(x_1')\;dx_1'=\delta_{\kappa\nu}}\\&=\sum_{\{\nu|\lambda_\nu<\Lambda\}}\psi_\nu(x_1)\psi_\nu^*(x_2)\end{aligned} \tag{E.31}$$

and

$$[\hat{a}_{x_1}^{(\Lambda)},\hat{a}_{x_2}^{(\Lambda)}]=0 \tag{E.32}$$

of the coarse grained ladder operators follow straightforwardly from the commutation relations (2.1) of the original ladder operators. The auxiliary calculation

$$\begin{aligned}\langle 0|\,\hat{a}_{x_1}^{(\Lambda)}\cdots\hat{a}_{x_I}^{(\Lambda)}\hat{a}_x^{(\Lambda)\dagger}&=\langle 0|\,[\hat{a}_{x_1}^{(\Lambda)}\cdots\hat{a}_{x_I}^{(\Lambda)},\hat{a}_x^{(\Lambda)\dagger}]\\&=\langle 0|\,[\hat{a}_{x_1}^{(\Lambda)}\cdots\hat{a}_{x_{I-1}}^{(\Lambda)},\hat{a}_x^{(\Lambda)\dagger}]\hat{a}_{x_I}^{(\Lambda)}+\langle 0|\,\hat{a}_{x_1}^{(\Lambda)}\cdots\hat{a}_{x_{I-1}}^{(\Lambda)}[\hat{a}_{x_I}^{(\Lambda)},\hat{a}_x^{(\Lambda)\dagger}]\\&\;\;\vdots\\&=\langle 0|\sum_{i=1}^I\hat{a}_{x_1}^{(\Lambda)}\cdots\hat{a}_{x_{i-1}}^{(\Lambda)}[\hat{a}_{x_i}^{(\Lambda)},\hat{a}_x^{(\Lambda)\dagger}]\hat{a}_{x_{i+1}}^{(\Lambda)}\cdots\hat{a}_{x_I}^{(\Lambda)}\\&=\sum_{i=1}^I\sum_{\{\nu|\lambda_\nu<\Lambda\}}\psi_\nu(x_i)\psi_\nu^*(x)\,\langle 0|\prod_{j\in\{1\cdots I\}\setminus\{i\}}\hat{a}_{x_j}^{(\Lambda)}\end{aligned}$$

is carried out, where the left out steps are an induction by I. Applying this calculation twice yields the second auxiliary calculation

$$\begin{aligned}&\langle 0|\,\hat{a}_{x_1}^{(\Lambda)}\cdots\hat{a}_{x_I}^{(\Lambda)}\hat{a}_x^{(\Lambda)\dagger}\hat{a}_{x'}^{(\Lambda)\dagger}\\&=\sum_{i=1}^I\sum_{\{\nu|\lambda_\nu<\Lambda\}}\psi_\nu(x_i)\psi_\nu^*(x)\,\langle 0|\left(\prod_{j\in\{1\cdots I\}\setminus\{i\}}\hat{a}_{x_j}^{(\Lambda)}\right)\hat{a}_{x'}^{(\Lambda)\dagger}\\&=\sum_{\substack{i,i'=1\\i'\neq i}}^I\sum_{\{\nu|\lambda_\nu<\Lambda\}}\psi_\nu(x_i)\psi_\nu^*(x)\sum_{\{\nu'|\lambda_\nu<\Lambda\}}\psi_{\nu'}(x_{i'})\psi_{\nu'}^*(x')\,\langle 0|\prod_{j\in\{1\cdots I\}\setminus\{i,i'\}}\hat{a}_{x_j}^{(\Lambda)}.\end{aligned}$$

With the help of the auxiliary calculations the linear form in the I-particle Schrödinger equation (E.30) evaluates to

$$
\begin{aligned}
&\langle 0|\,\hat{a}^{(\Lambda)}_{x_1}\cdots\hat{a}^{(\Lambda)}_{x_I}\hat{H}_\Lambda\\
=&\int\limits_M \langle 0|\,\hat{a}^{(\Lambda)}_{x_1}\cdots\hat{a}^{(\Lambda)}_{x_I}\hat{a}^{(\Lambda)\dagger}_{x}\frac{-\hbar^2}{2m}\Delta\hat{a}^{(\Lambda)}_{x}\;dx+\frac{1}{2}\int\limits_M\int\limits_M \langle 0|\,\hat{a}^{(\Lambda)}_{x_1}\cdots\hat{a}^{(\Lambda)}_{x_I}\hat{a}^{(\Lambda)\dagger}_{x}\hat{a}^{(\Lambda)\dagger}_{x'}V(x{-}x')\hat{a}^{(\Lambda)}_{x}\hat{a}^{(\Lambda)}_{x'}\;dx\;dx'\\
=&\sum_{i=1}^{I}\sum_{\{\nu|\lambda_\nu<\Lambda\}}\psi_\nu(x_i)\int\limits_M dx\;\psi^*_\nu(x)\frac{-\hbar^2}{2m}\Delta_x\,\langle 0|\,\hat{a}^{(\Lambda)}_{x}\prod_{j\in\{1\cdots I\}\setminus\{i\}}\hat{a}^{(\Lambda)}_{x_j}\\
&+\frac{1}{2}\sum_{\substack{i,i'=1\\ i'\neq i}}^{I}\sum_{\{\nu|\lambda_\nu<\Lambda\}}\psi_\nu(x_i)\int\limits_M dx\;\psi^*_\nu(x)\sum_{\{\nu'|\lambda'_\nu<\Lambda\}}\psi_{\nu'}(x_{i'})\int\limits_M dx'\;\psi^*_{\nu'}(x')V(x{-}x')\,\langle 0|\,\hat{a}^{(\Lambda)}_{x}\hat{a}^{(\Lambda)}_{x'}\prod_{j\in\{1\cdots I\}\setminus\{i,i'\}}\hat{a}^{(\Lambda)}_{x_j}\\
=&\left(\sum_{i=1}^{I}C_{\Lambda x_i}\frac{-\hbar^2}{2m}\Delta_{x_i}+\frac{1}{2}\sum_{\substack{i,i'=1\\ i'\neq i}}^{I}C_{\Lambda x_i}C_{\Lambda x_{i'}}V(x_i-x_{i'})\right)\hat{a}^{(\Lambda)}_{x_1}\cdots\hat{a}^{(\Lambda)}_{x_I}.
\end{aligned}
\tag{E.33}
$$

In the last equality, an additional subscript was added to the coarse graining operator to indicate on which variable it acts like $C_{\Lambda x_i}f(x_1,\cdots x_I)\equiv C_\Lambda\left(f(x_1,\cdots x_{i-1},\bullet,x_{i+1}\cdots x_I)\right)(x_i)$.

Inserting this result into the Schrödinger equation (E.30) yields

$$
i\hbar\frac{d}{dt}\psi(x_1,\cdots x_I,t)=\left(\sum_{i=1}^{I}C_{\Lambda x_i}\frac{-\hbar^2}{2m}\Delta_{x_i}+\frac{1}{2}\sum_{\substack{i,i'=1\\ i'\neq i}}^{I}C_{\Lambda x_i}C_{\Lambda x_{i'}}V(x_i-x_{i'})\right)\psi(x_1,\cdots x_I,t).
\tag{E.34}
$$

As C_Λ is a projection into a subspace of eigenvectors of the Laplace-Beltrami operator, the two commute. Additionally, due to the projection property $C_\Lambda^2=C_\Lambda$, the coarse graining operator does not change the wavefunction ψ when acting on it, i.e.

$$
C_{\Lambda x_i}\psi(x_1,\cdots x_I,t)=C_{\Lambda x_i}\left(\prod_{i'=1}^{I}C_{\Lambda x_{i'}}\right)\big\langle 0\big|\hat{a}_{x_1}\cdots\hat{a}_{x_I}\big|\Psi(t)\big\rangle=\psi(x_1,\cdots x_I,t).
\tag{E.35}
$$

Consequently, C_Λ is interchanged with Δ and then omitted in the I-particle Schrödinger equation (E.36) of the coarse grained system, which thereby simplifies to

$$
i\hbar\frac{d}{dt}\psi(x_1,\cdots x_I,t)=\left(\sum_{i=1}^{I}\frac{-\hbar^2}{2m}\Delta_{x_i}+\frac{1}{2}\sum_{\substack{i,i'=1\\ i'\neq i}}^{I}C_{\Lambda x_i}C_{\Lambda x_{i'}}V(x_i-x_{i'})\right)\psi(x_1,\cdots x_I,t).
\tag{E.36}
$$

Quantum statistics It is briefly discussed, how the coarse graining impacts the quantum statistical considerations made in section 3.1. There, a simplified expression for the grand canonical potential is derived, starting out with transformations of the thermal energy operator $\hat{T}$. In the first transformation of $\hat{T}$, the spatial dependence of the ladder operators is expanded into a series over a set of eigenfunctions of the Laplace-Beltrami operator. For the coarse grained system, $\hat{T}$ depends on the coarse grained ladder operators $\hat{a}^{(\Lambda)}_x$ instead of the original $\hat{a}_x$. By definition of the coarse graining operator, its action on the function of ladder operator $\hat{a}_\bullet$ also amounts to such an expansion, except leaving out contributions of the eigenfunctions with low eigenvalues. Consequently, for the coarse grained system, instead of the expression (3.14) for $\hat{T}$, one gets the same expression, except with the summation over the quantum numbers running only over the set $\{\nu|\lambda_\nu<\Lambda\}$. That means, that all subsequent calculations in section 3.1 work identically for the coarse grained system. The only necessary adaption is restricting any previously unrestricted summations over the quantum numbers to the set $\{\nu|\lambda_\nu<\Lambda\}$. In particular, the quantum fluctuations in the final expressions (3.83) for the ground state occupation and (3.85) for the grand-canonical potential become finite due to the coarse graining. In the super-canonical treatment of the Bose gas in a box in section 3.2, the divergent quantum fluctuations are regularized by approximating the summation over the

quantum numbers by an integration (3.106) and introducing a cutoff in the radial integral. This precise cutoff is now a natural feature of the coarse grained description and therefore eliminates the necessity for regularization.

Scattering theory The effect of the coarse graining on the scattering theory discussed in section D is less trivial. The scattering theory deals with the two-particle description of free particles with pairwise interaction mediated by V. The equation of motion of the scattering theory of the coarse grained system is derived. The above derivation of the I-particle Schrödinger equation (E.36) works identically for the case $M = \mathbb{R}^n$ by using the "continuous" version (E.16) of the coarse graining operator. Specializing on $I = 2$ in (E.36) then yields

$$i\hbar\frac{d}{dt}\psi(x_1,x_2,t) = \left(\frac{-\hbar^2}{2m}\Delta_{x_1} + \frac{-\hbar^2}{2m}\Delta_{x_2} + C_{\Lambda x_1}C_{\Lambda x_2}V(x_1-x_2)\right)\psi(x_1,x_2,t), \tag{E.37}$$

which only differs from its analogon (D.2) in the pair $C_{\Lambda x_1}C_{\Lambda x_2}$ of coarse graining operators acting on the product $V(x_1 - x_2)\psi(x_1, x_2, t)$.

In the scattering theory of the original system, the first step in solving the Schrödinger equation is switching to the center of mass coordinate frame (D.14) via the transformation (D.15) of the wavefunction. For the coarse grained system, this step is influenced by the presence of the coarse graining operators in Equation (E.37). To simplify the notation, one abbreviates $f(x_1, x_2) = V(x_1 - x_2)\psi(x_1, x_2, t)$ for any fixed value of t. Therewith, the action of the coarse graining operators on the product of V and ψ is expanded into

$$\begin{aligned}
&C_{\Lambda x_1}C_{\Lambda x_2}f(x_1,x_2)\\
=&C_{\Lambda x_1}(2\pi)^{-n}\int\limits_{B_\Lambda(0)} dk_2\; e^{ik_2\cdot x_2}\int\limits_{\mathbb{R}^n} dx'\; {}_2e^{-ik_2\cdot x_2'}f(x_1,x_2')\\
=&(2\pi)^{-2n}\int\limits_{B_\Lambda(0)} dk_1\int\limits_{B_\Lambda(0)} dk_2\; e^{i(k_1\cdot x_1+k_2\cdot x_2)}\int\limits_{\mathbb{R}^n} dx_1'\int\limits_{\mathbb{R}^n} dx_2'\; e^{-i(k_1\cdot x_1'+k_2\cdot x_2')}f(x_1',x_2')\\
=&(2\pi)^{-2n}\int\limits_{B_\Lambda(0)} dk_1\int\limits_{B_\Lambda(0)} dk_2\; e^{i(k_1\cdot x_1+k_2\cdot x_2)}\int\limits_{\mathbb{R}^n} dx'\int\limits_{\mathbb{R}^n} dX'\; e^{-i(k_1\cdot(X'+\frac{x'}{2})+k_2\cdot(X'-\frac{x'}{2}))}f\left(X'+\frac{x'}{2},X'-\frac{x'}{2}\right).
\end{aligned} \tag{E.38}$$

For the last equality, the substition $x' = x_1' - x_2'$ and $X' = \frac{x_1'+x_2'}{2}$ of center of mass-coordinates was performed, which notably has the constant volume element 1. Introducing the new abbreviation $f'(x, X) \equiv f(X + \frac{x}{2}, X - \frac{x}{2}) = V(x)\psi(X + \frac{x}{2}, X - \frac{x}{2}, t)$, this equation is evaluated in the center of mass frame, which gives

$$\begin{aligned}
&\left(C_{\Lambda x_1}C_{\Lambda x_2}f(x_1,x_2)\right)\Big|_{\substack{x_1=X+\frac{x}{2}\\ x_2=X-\frac{x}{2}}}\\
=&(2\pi)^{-2n}\int\limits_{B_\Lambda(0)} dk_1\int\limits_{B_\Lambda(0)} dk_2\int\limits_{\mathbb{R}^n} dx'\int\limits_{\mathbb{R}^n} dX'\; e^{i(k_1+k_2)\cdot(X-X')}e^{i\frac{k_1-k_2}{2}\cdot(x-x')}f(x',X')\\
=&(2\pi)^{-2n}\int\limits_{B_\Lambda(0)} dk\int\limits_{S} dK\int\limits_{\mathbb{R}^n} dx'\int\limits_{\mathbb{R}^n} dX'\; e^{iK\cdot(X-X')}e^{ik\cdot(x-x')}f(x',X').
\end{aligned} \tag{E.39}$$

For the last equality, the substition $k = \frac{k_1-k_2}{2}$ and $K = k_1+k_2$ was performed. The possible values for the transformed variables are $k \in B_\Lambda(0)$ and $K \in B_{2\Lambda}(0)$, but aren't adopted independently. Instead, for any $k \in B_\Lambda(0)$, the integration with respect to K runs over the set $S \equiv \{K \in \mathbb{R}^n | \exists k_1, k_2 \in B_\Lambda(0) : k = \frac{k_1-k_2}{2} \wedge K = k_1 + k_2\}$. The set S does at least contain the ball with radius $\Lambda - \|k\|$, i.e. $B_{\Lambda-\|k\|}(0) \subset S$ due to the consideration

$$\|K\| < 2(\Lambda - \|k\|) \Rightarrow \Lambda > \|k\| + \frac{1}{2}\|K\| \geq \begin{cases} \|\frac{K}{2} + k\| = \|k_1\| \\ \|\frac{K}{2} - k\| = \|k_2\| \end{cases}. \tag{E.40}$$

Equation (E.39) is rewritten as

$$\left(C_{\Lambda x_1} C_{\Lambda x_2} f(x_1, x_2)\right)\Big|_{\substack{x_1 = X + \frac{x}{2} \\ x_2 = X - \frac{x}{2}}} = C_{\Lambda x} C_{2\Lambda X} f'(x, X) + r_\Lambda(x, X) \tag{E.41}$$

with the remainder

$$r_\Lambda(x, X) = (2\pi)^{-2n} \int\limits_{B_\Lambda(0)} dk \int\limits_{\mathbb{R}^n} dx' \; e^{ik\cdot(x-x')} \int\limits_{B_{2\Lambda}(0)\setminus S} dK \int\limits_{\mathbb{R}^n} dX' \; e^{iK\cdot(X-X')} f(x', X'). \tag{E.42}$$

Without further investigation, it is assumed that this remainder vanishes in the limit $\Lambda \to \infty$ and it is discarded. Therefore and by writing out the abbreviations f and f', Equation (E.41) reduces to

$$\left(C_{\Lambda x_1} C_{\Lambda x_2} V(x_1 - x_2)\psi(x_1, x_2, t)\right)\Big|_{\substack{x_1 = X + \frac{x}{2} \\ x_2 = X - \frac{x}{2}}} \approx C_{\Lambda x} C_{2\Lambda X} V(x)\psi(X + \frac{x}{2}, X - \frac{x}{2}, t). \tag{E.43}$$

Expressing this equation in words in an oversimplified manner, the two coarse graining operators approximately commute with the transformation to center of mass coordinates. For the coarse grained system, switching to center of mass coordinates consequently entails the differential equation

$$\left(-\frac{\hbar^2}{4m}\Delta_X - \frac{\hbar^2}{m}\Delta_x + C_{\Lambda x} V(x)\right)\psi(X + \frac{x}{2}, X - \frac{x}{2}, t) = i\hbar\frac{d}{dt}\psi(X + \frac{x}{2}, X - \frac{x}{2}, t), \tag{E.44}$$

which is the analogon to Equation (D.16). Then, the separation of the variables x, X and t is performed with a product ansatz analogous to (D.17). For the multiplicative component ϕ of the wavefunction that depends on the relative coordinates x, one gets the differential equation

$$\left(-\frac{\hbar^2}{m}\Delta_x + C_{\Lambda x} V(x)\right)\phi(x) = (E - E')\phi(x), \tag{E.45}$$

in contrast to Equation (D.20) for the original system. Rewriting this differential equation as the Lippmann-Schwinger equation yields

$$\begin{aligned} \phi_{\text{sca}}(x) =& \int\limits_{\mathbb{R}^n} G_\kappa(x - x')\frac{m}{\hbar^2} C_\Lambda(V\phi)(x') \; dx' \\ =& \frac{m}{\hbar^2} C_\Lambda(V\phi) * G_\kappa \\ =& \frac{m}{\hbar^2}(V\phi) * C_\Lambda(G_\kappa) \\ =& \int\limits_{\mathbb{R}^n} C_\Lambda\left(G_\kappa\right)(x - x')\frac{m}{\hbar^2} V(x')\phi(x') \; dx' \end{aligned} \tag{E.46}$$

for the scattered wave, which only differs from its analogon (D.22) in the coarse graining operator acting on the Greens' function G_κ. The third equality is due to the auxiliary result

$$\begin{aligned} f * C_\Lambda(g) =& \mathcal{F}(\mathcal{F}^{-1}(f)) * \mathcal{F}(1_{B_\Lambda(0)}\mathcal{F}^{-1}(g)) \\ =& \mathcal{F}(\mathcal{F}^{-1}(f)1_{B_\Lambda(0)}\mathcal{F}^{-1}(g)) \\ =& \mathcal{F}(1_{B_\Lambda(0)}\mathcal{F}^{-1}(f)) * \mathcal{F}(\mathcal{F}^{-1}(g)) = C_\Lambda(f) * g, \end{aligned}$$

which is in turn based on the convolution theorem $\mathcal{F}(f) * \mathcal{F}(g) = \mathcal{F}(fg)$. The remaining considerations on the scattering theory in section D play out identically for the coarse grained system, because they only depend on the far field behaviour of the Greens' function, which is unaltered by the coarse graining operator for $\Lambda > \kappa$.

In the beginning of section 3.2.2, the relation between the interaction strength g and the s-wave scattering length a_s is derived for the original system. There, the divergence of the inverse scattering length emerges due to the evaluation (3.102) of the Greens' function G_κ at the origin, which is then regualrized by introducing a cutoff to the radial integral. For the coarse grained system on the other hand, due to Equation (E.46), $C_\Lambda(G_\kappa)$ is evaluated at the origin instead. From the general expression (D.5) for the Greens' function of the Helmoltz operator, one gets

$$C_\Lambda(G_\kappa)(x-x') = \mathcal{F}^{-1}\left(I_\Lambda \mathcal{F}\left(\mathcal{F}^{-1}\left(\frac{(2\pi)^{-\frac{n}{2}}}{\kappa^2 - \|\bullet\|^2}\right)\right)\right)(x-x') = (2\pi)^{-n} \int\limits_{B_\Lambda(0)} \frac{e^{iq\cdot(x-x')}}{\kappa^2 - \|q\|^2}\, dq. \quad \text{(E.47)}$$

The cutoff, which has to be introduced manually in Equation (3.102) for the original system, therefore arises naturally in the treatment of the coarse grained system. The regularization of the inverse interaction strength is consequently unnecessary.

To summarize, the impact of the coarse graining of the quantum mechanical model influences both the scattering theory and the quantum statistcs in a way, that prevents the emergence of ultra violet divergencies, which would normally arise due to approximating the two-particle interaction by contact interaction. The heuristic regularization scheme of subtracting infinities is thereby given a mathematically rigorous foundation.

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