

Influence of the Exchange Symmetry beyond the Exclusion Principle



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Abstract

Since typically the physics of many body quantum systems is solely described and determined by pairwise interactions, the concept of reduced particle information is fundamentally relevant, particularly for indistinguishable particles. Determining the compatibility of r -particle reduced density operators (r -RDOs) with some N -particle state is known as the N -representability problem. The Pauli exclusion principle provides a set of necessary and sufficient conditions for the N -representability of fermionic 1-RDOs. However, pure N -representability requires a set of stricter conditions which are known as Generalised Pauli constraints (GPCs).

In this thesis we investigate the influence and significance of the GPCs *beyond* the well-explored and established relevance of the Pauli exclusion principle. In particular, we *analytically* study the (quasi-)pinning effect which corresponds to a saturation of the GPCs and imposes structural simplifications on the N -fermion state. So far, nothing is known about its origin and mechanisms. We will close this gap by analytically examining the dependence of quasipinning on the particle number, the dimensionality and the spin polarisation in a representative physical model system. Our results suggest the notion of a microscopic Pauli pressure which is a consequence of the competition between energy minimisation and antisymmetry, and drives the system towards the boundary of the allowed region. Furthermore, the relevance of quasipinning beyond the well-known Pauli exclusion principle is evaluated by the Q -measure. The outcomes provide first direct evidence for the need to incorporate GPCs into the physical description.

To explore the role of the fermionic exchange symmetry beyond the Pauli exclusion principle from a more general perspective, we consider systems of hardcore bosons. Indeed, they exhibit a (lattice-based) exclusion principle, although their exchange symmetry is bosonic. Occupation numbers on one-particle states other than the lattice basis can exceed one. We prove that the maximal occupation number is given by $\lambda_{max} = N/d(d - N + 1)$ where N, d are the numbers of particles and lattice sites. In addition, we derive necessary conditions for the N -representability of hardcore boson 1-RDOs and investigate the one-particle entropy boundaries. Finally, we present *one-dimensional* physical systems which macroscopically saturate λ_{max} and exhibit (fractional) Bose-Einstein condensation.

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Chapter 1

Pauli's Exclusion Principle and beyond

The indistinguishability of identical particles is a fascinating and fundamentally important feature of quantum mechanics. It plays a crucial role in the physical mechanisms governing numerous systems such as atoms, solids and even astronomical objects like neutron stars. In particular, it was found responsible for the stability of matter itself [60, 61].

At the beginning of the 1920s, studies of the atomic structure revealed the *Aufbau principle*, which in 1925 prompted Pauli to postulate his famous *exclusion principle* [75]. Just one year later, Dirac and Heisenberg [30] showed that the Pauli exclusion principle could be considered merely a consequence of a more fundamental symmetry in nature: the antisymmetry of the many-fermion wave function under particle exchanges. The Pauli exclusion principle thus follows from the indistinguishability of fermions in the form of the spin-statistics theorem. Since then, numerous works have explored the nature of both fundamental particle species, bosons and fermions.

Many-fermion systems are frequently encountered in many branches of Physics and form the basis of Chemistry and Materials Science. Providing an efficient description for them has thus been an important objective of research for many decades. A major challenge, however, is posed by the complexity of the underlying Schrödinger equation, which grows exponentially with the size of the system.

In the 1950s, investigations into the concepts of reduced particle information raised hopes that an efficient description of many-fermion systems could be given in terms of one- and two-particle reduced density operators [26, 25]. This is because physical non-relativistic Hamiltonians only comprise 1- and 2-body terms $\hat{H}_1$ and $\hat{H}_2$. More specifically, it was noted that the energy functional of any such Hamiltonian $\hat{H}$ would solely depend on the two-particle reduced density operator ρ_2 , whose complexity

scales polynomially.

$$E = \text{tr}(\rho_N \hat{H}) = \text{tr}(\rho_2 \hat{H}_2). \quad (1.1)$$

The ground state of a system could therefore easily be determined by a variation over the domain of all those operators *compatible* with some N -particle state.

The question as to the compatibility of r -particle reduced density operators to N -fermion quantum states became also known as the *r -body N -representability problem*. This problem is a special type of the more general *quantum marginal problem*. In the important case of fermionic two-particle density operators it was named *Coulson's challenge*.¹ Unfortunately, the problem was recently shown to be Quantum Merlin-Arthur (QMA) complete [63], which suggests that it cannot be solved efficiently in the system's size, even by using a quantum computer.

By contrast, the fermionic one-body N -representability problem possesses a feasible solution. A set of necessary conditions is famously given by the Pauli exclusion principle of having no more than one fermion on any one-particle orbital. Although these conditions are also recognised sufficient for the N -representability by mixed states, it was unknown whether this would hold for pure states as well.

First evidence for the existence of further restrictions beyond the Pauli exclusion principle was found by Borland and Dennis in 1972 [12]. Only recently, the problem of fermionic pure one-body N -representability was solved in a series of remarkable works by Altunbulak and Klyachko [1, 2, 50, 51, 52]. They found that necessary and sufficient conditions were given by a set of linear inequalities on the eigenvalues of the one-particle reduced density operator, which now became known as Generalised Pauli constraints. This further showed that the fermionic antisymmetry is a stronger constraint than the exclusion principle.

In this thesis, we study the role of the particle exchange symmetry in the form of the Generalised Pauli constraints, and try to determine its influence *beyond* the weaker Pauli exclusion principle. Because the Pauli exclusion principle is known to be of fundamental importance to our understanding of various physical systems, stronger constraints can be expected to be of even greater physical significance. The behaviour of fermionic systems heavily depends on the competition between the fermionic antisymmetry and energy minimisation. Hence, one can expect the fermionic antisymmetry to play a crucial role whenever some of the Generalised Pauli constraints

¹The national research council of the United States identified Coulson's challenge as one of the ten most important problems in Quantum Chemistry [27].

are (approximately) saturated. This effect was coined as (quasi-)pinning by Klyachko [52] and Schilling [87], and has seen a growing interest over the past few years [52, 7, 53, 87, 18, 84, 86, 9, 96, 64, 85].

One of the first analytical treatments [87] revealed a strong approximate saturation of the Generalised Pauli constraints in a system of three harmonically interacting particles confined in a one-dimensional external harmonic potential. However, little if anything was known about the mechanisms and the general origin of this quasipinning. Therefore, we systematically study the quasipinning of various physical model systems and consider in detail the influence of the particle number, dimensionality and spin polarisation on the quasipinning. The different ground states of these systems emerge due to the competition between the energy minimisation and the antisymmetry of the fermionic wave function and thereby unveil the mechanism behind quasipinning.

In order to evaluate the relevance of these results beyond what could be expected from the weaker Pauli exclusion principle, we apply the Q -measure recently developed by Schilling [94]. We find that quasipinning strongly relies on the ‘active space’ structure around the Fermi level. Increasing the number of particles and the degree of spin polarisation, as well as decreasing the dimensionality yields a larger saturation of the constraints which can be interpreted by the notion of a ‘microscopic Pauli pressure’. The Q -parameter of these systems confirms the relevance of the Generalised Pauli constraints beyond the exclusion principle.

In a second and different approach we consider hardcore bosons to study the role of the exclusion principle in systems with bosonic instead of fermionic exchange symmetry. Hardcore bosons are particles which obey bosonic commutation relations and exert a large particle-particle on-site interaction on one another. This gives rise to a dynamically imposed exclusion principle for hardcore bosons on the lattice sites. We will implement this analogue of the Pauli exclusion principle as a kinematical constraint by restricting the N -boson Hilbert space to the smaller N -hardcore boson Hilbert space. In contrast to fermions, the hardcore boson exclusion principle only holds in a specific lattice basis. We will prove a theorem which constitutes an upper bound λ_{max} on one-particle hardcore boson occupation numbers. The maximal occupation number is found to depend on the number of particles N and lattice sites d only:

$$\lambda_{max} = \frac{N}{d} (d - N + 1) . \quad (1.2)$$

Equipped with this structural insight we study the one-body N -representability problem for hardcore bosons. Since in many hardcore boson systems the on-site interaction is the only two-body term in the Hamiltonian, the knowledge about the set of all

compatible one-particle density operators would allow for an efficient description of many-body hardcore boson systems. Similar to fermions the reason for this is given by a significantly simplified form of the energy functional, which in the case of various hardcore boson systems will solely depend on the 1-RDO. We will determine necessary conditions for the hardcore boson one-body N -representability of systems with arbitrary numbers of particles and lattice sites. In addition, we will examine different one-particle entropy measures. Our results provide evidence for a hybrid character of hardcore bosons. Finally we will investigate two physical systems which exhibit hardcore boson pinning, i.e. the saturation of the previously determined conditions for N -representability.

The thesis is mainly structured in the following three parts:

Chapter 2 In the second chapter, we briefly review the concepts of many-body quantum mechanics and introduce the conventions and notations used throughout this thesis. We will define the N -representability problem and discuss its particular solution in terms of Generalised Pauli constraints. Furthermore, we will present the methods and tools required for the analyses in the third chapter. In particular, we will review the quasipinning phenomenon and the Q -measure.

Chapter 3 In the third chapter, the results of the author's research on the realm of quasipinning will be presented. We will introduce the physical model system of Harmonium and determine analytically its ground state for various particle numbers and spatial dimensions. This will be followed by various (quasi-)pinning analyses for systems of different particle numbers, different dimensionalities, including dimensional crossovers, and different spin polarisations.

Chapter 4 In the fourth chapter, we present the result on the author's research on the one-body N -representability problem for hardcore bosons. We will start by proving a theorem on the maximal one-particle occupation number and discuss the structural properties of the maximising state. Next, we will derive necessary conditions for the one-particle N -representability. Then we will discuss bounds on one-particle entropy measures. Finally, we consider two systems whose ground states saturate the maximal occupation number and exhibit fractional Bose-Einstein condensation.

In the fifth chapter, we will summarise and discuss the results of this thesis. Selected supporting information will be provided in the appendix.

The results of the author's research presented in the third chapter have also been published in Refs. [94, 93, 95].

Chapter 2

Many-body quantum systems, fermionic N -representability and the Q -parameter

2.1 Exposition

In this chapter we briefly review the language and key concepts of many-body quantum physics. This will allow us to set up the notations and conventions which will be applied throughout the rest of this thesis.

We shall start by considering N -particle systems of bosons and fermions in Sec. 2.2. This will be followed by an introduction of the concept of reduced particle information in the form of reduced density operators. We shall discuss the physical relevance of these operators. In particular, we shall see that one- and two-particle reduced density operators give rise to a powerful structural simplification of the related physical energy functionals. In order to make use of these functionals and reduce the complexity of the description of many-body quantum systems, one has to solve the so-called N -representability problem.

We shall define this problem and present two theorems on the N -fermion compatibility of one-particle density operators in Sec. 2.3. A set of necessary conditions is given by the famous Pauli exclusion principle. These conditions, however, are not always sufficient. For pure N -fermion states, a set of necessary *and* sufficient conditions is given by the so-called Generalised Pauli constraints, which are more restrictive than the Pauli exclusion principle. The saturation of these constraints, which mathematically arise from the intrinsic nature of N -fermion states, is called the pinning effect. In order to allow for an investigation of this effect in the third chapter, we shall introduce the required techniques.

For that, we shall review the concept of a truncated pinning analysis [87, 84] in Sec. 2.4. In the last section, we shall report on the Q -measure which has recently been developed in Ref. [94]. This measure provides a means to quantify the relevance of the Generalised Pauli constraints beyond the influence of the well-known Pauli exclusion principle in N -fermion systems.

2.2 N -particle Quantum Systems: Framework and notational conventions

The quantum mechanical description of a single particle is based on the notion of the d -dimensional¹ one-particle Hilbert space $\mathcal{H}_1^{(d)}$ and unitary evolution in time. A distinction is made between *pure* physical states represented by a vector $|\phi\rangle \in \mathcal{H}_1^{(d)}$ and *mixed* physical states, which are represented by hermitian, positive-semidefinite trace-1-class operators on the Hilbert-Schmidt space $\mathcal{HS}(\mathcal{H}_1^{(d)})$ of bounded linear operators on $\mathcal{H}_1^{(d)}$. The set of mixed states forms the closed convex hull of the set of pure state density operators $\rho = |\varphi\rangle\langle\varphi|$. Famously, the unitary evolution operator $\hat{U}$ is determined by the Schrödinger equation:

$$i\hbar \frac{d}{dt} \hat{U}(t) = \hat{H} \hat{U}, \quad (2.1)$$

which depends on the Hamiltonian $\hat{H}$ of the specific physical system at hand.

Many-particle concepts

For N distinguishable particles this framework can be generalised by introducing the N -particle Hilbert space, which for N identical one-particle Hilbert spaces is commonly written as:

$$\mathcal{H}_N \equiv \underbrace{\mathcal{H}_1^{(d)} \otimes \dots \otimes \mathcal{H}_1^{(d)}}_{N\text{-times}} \equiv \left(\mathcal{H}_1^{(d)}\right)^{\otimes N}. \quad (2.2)$$

(Elementary) particles with identical properties, i.e. equal mass, charge, intrinsic spin, colour, etc., can in principle not be distinguished from one another. The physical description must reflect this by remaining invariant under the operation of swapping any two particles. The exchange of particles i and j possesses a unitary representation $\hat{\mathcal{U}}_{i \leftrightarrow j}$ acting on $\mathcal{H}_N$. Applying this transformation twice to a system

¹ $d \in \{\mathbb{N} \cup \infty\}$.

with a 3-dimensional single-particle configuration space equals the identity operation.² Therefore, $\hat{\mathcal{U}}_{i \leftrightarrow j}$ has eigenvalues ± 1 . In nature, one can correspondingly find two species of particles with definite exchange symmetry: bosons and fermions. N -boson and N -fermion states are positive and negative eigenstates of all $N(N-1)/2$ pair-swapping transformations $\hat{\mathcal{U}}_{i \leftrightarrow j}$, respectively. If some N -particle Hamiltonian is invariant under particle exchanges, its associated N -particle system can be regarded as a bosonic or fermionic system. The Hilbert space of the quantum mechanical description then has to be restricted to the subspace of either totally symmetric or antisymmetric states, i.e. states with positive or negative exchange symmetry. We shall now define the projectors onto these subspaces.

Bosonic and Fermionic Hilbert Spaces

Let S_N denote the group of all permutations of N elements. A unitary representation of the permutation group acting on $\mathcal{H}_N$ may be found by successively applying the particle swapping operations $\hat{\mathcal{U}}_{i \leftrightarrow j}$. The unitary $\hat{\mathcal{U}}_\sigma$, which represents the permutation $\sigma \in S_N$, is a linear operator whose action on a product of single particle states $|\phi_i\rangle \in \mathcal{H}_1^{(d)}$ is given by:

$$\hat{\mathcal{U}}_\sigma[|\phi_1\rangle \otimes |\phi_2\rangle \otimes \dots \otimes |\phi_N\rangle] := |\phi_{\sigma^{-1}(1)}\rangle \otimes |\phi_{\sigma^{-1}(2)}\rangle \otimes \dots \otimes |\phi_{\sigma^{-1}(N)}\rangle. \quad (2.3)$$

The projectors onto the bosonic and fermionic subspaces of $\mathcal{H}_N$ are the symmetrising operator $\mathcal{S}_N$ and the antisymmetrising operator $\mathcal{A}_N$, defined by:

$$\mathcal{S}_N |\Psi_N\rangle = \frac{1}{\sqrt{N!}} \sum_{\sigma \in S_N} \hat{\mathcal{U}}_\sigma |\Psi_N\rangle, \quad (2.4a)$$

$$\mathcal{A}_N |\Psi_N\rangle = \frac{1}{\sqrt{N!}} \sum_{\sigma \in S_N} \text{sign}(\sigma) \hat{\mathcal{U}}_\sigma |\Psi_N\rangle. \quad (2.4b)$$

Consequently, the fermionic and bosonic subspaces can be expressed as:

$$\mathcal{H}_N^{(f)} \equiv \mathcal{A}_N[\mathcal{H}_N] \equiv \wedge^N [\mathcal{H}_1^{(d)}] \leq \mathcal{H}_N \quad (2.5)$$

and

$$\mathcal{H}_N^{(b)} \equiv \mathcal{S}_N[\mathcal{H}_N] \leq \mathcal{H}_N. \quad (2.6)$$

In the language of density operators, a mixed N -fermion state $\rho_N^{(f)}$ has to fulfil the following conditions:

$$\rho_N^{(f)} = \mathcal{A}_N \rho_N^{(f)} = \rho_N^{(f)} \mathcal{A}_N. \quad (2.7)$$

²Note that this is not true in strictly two-dimensional systems in which the different topology of the configuration space gives rise to fractional statistics and the occurrence of anyonic quasi-particles; see Ref. [89] for more information.

Similarly, projective relations are found for mixed bosonic states. The convex sets of mixed fermionic and bosonic density operators shall be denoted by $\mathcal{M}_N^{(f)}$ and $\mathcal{M}_N^{(b)}$:

$$\begin{aligned}\mathcal{M}_N^{(f)} &:= \{\rho_N \in \mathcal{HS}(\mathcal{H}_N) \mid \rho_N = \mathcal{A}_N \rho_N = \rho_N \mathcal{A}_N, \text{ tr}(\rho_N) = 1, \rho_N \geq 0\}; \\ \mathcal{M}_N^{(b)} &:= \{\rho_N \in \mathcal{HS}(\mathcal{H}_N) \mid \rho_N = \mathcal{S}_N \rho_N = \rho_N \mathcal{S}_N, \text{ tr}(\rho_N) = 1, \rho_N \geq 0\}.\end{aligned}\quad (2.8)$$

Reduced Density Operators

The full information encoded in $\rho_N^{(f/b)}$ about N indistinguishable particles is usually not required for understanding many physical properties of a system at hand. Considering only the reduced information about a smaller number of particles thus provides a crucial concept. For that purpose, one has to introduce the partial trace.

Let $\{|j_i\rangle\}_{j_i=0}^{d_i-1}$ be an orthonormal basis of $\{\mathcal{H}_{1,i}^{(d_i)}\}$, which induces the product basis $|j_1\rangle \otimes |j_2\rangle \otimes \dots \otimes |j_N\rangle$, $j_i \in \{0, \dots, d_i - 1\}$, on the N -particle Hilbert space $\mathcal{H}_N$. Denote the components of the N -particle density operator ρ_N in that basis by $(\rho_N)_{j_1, \dots, j_N, j'_1, \dots, j'_N}$. The reduced $(N-1)$ -particle density operator $\rho_{N \setminus \{k\}}$ is derived by tracing out the k^{th} particle of ρ_N . Its components in the product basis of $\{|j_i\rangle\}_{j_i=0}^{d_i-1}$ are given by

$$(\rho_{N \setminus \{k\}})_{j_1, \dots, j_{k-1}, j_{k+1}, \dots, j_N, j'_1, \dots, j'_{k-1}, j'_{k+1}, \dots, j'_N} = \sum_{j_k=1}^{d_k} \delta_{j_k j'_k} (\rho_N)_{j_1, \dots, j_N, j'_1, \dots, j'_N}. \quad (2.9)$$

The partial trace is a linear operation and can therefore be restricted to the bosonic and fermionic subspaces of $\mathcal{H}_N$. For states of indistinguishable particles, the partial trace becomes independent of the traced out particle index:

$$\text{tr}_{\{k\}}[\rho_N^{(f/b)}] = \text{tr}_{\{m\}}[\rho_N^{(f/b)}], \quad \forall m, k \in \{1, \dots, N\}. \quad (2.10)$$

The partial trace over multiple particles can be defined by repeatedly applying the partial trace over a single particle:

$$\rho_{N \setminus \{k_1, \dots, k_r\}} := \text{tr}_{\{k_1\}} \circ \text{tr}_{\{k_2\}} \circ \dots \circ \text{tr}_{\{k_r\}}[\rho_N]. \quad (2.11)$$

Due to the independence of the partial trace on the particle label in an ensemble of indistinguishable particles (2.10), the partial traces of $\rho_N^{(f/b)}$ can be defined merely by the number of the particles to be traced out. Without loss of generality, this may conveniently be written as:

$$\rho_r^{(f/b)} \equiv \text{tr}_{N-r}[\rho_N] := \rho_{N \setminus \{k_1, \dots, k_{N-r}\}}^{(f/b)}. \quad (2.12)$$

Henceforth, $\rho_r^{(f/b)}$ shall be called the r -particle (reduced) density operator (r-RDO) of the N -particle density operator $\rho_N^{(f/b)}$. In order to present and discuss various concepts and relations of r -particle density operators, it proves helpful to use the language of second quantisation, i.e. Fock spaces and ladder operators.

Fock spaces and ladder operators

So far we have considered Hilbert spaces of systems with fixed particle number. Additional powerful tools - also applicable to systems with constant particle number - can be provided by allowing for variable particle numbers, which in turn requires the introduction of the Fock spaces $\mathcal{F}^{(f/b)}$:

$$\mathcal{F}^{(f)} := \bigoplus_{N=0}^d \mathcal{A}_N[\mathcal{H}_N]. \quad (2.13)$$

Recall that d represents the dimension of the underlying one-particle Hilbert space. Similarly, the Fock space for bosons can be constructed as an infinite direct sum of N -particle Bosonic Hilbert spaces:

$$\mathcal{F}^{(b)} := \bigoplus_{N=0}^{\infty} \mathcal{S}_N[\mathcal{H}_N]. \quad (2.14)$$

The Fock spaces can be equipped with a basis induced by an orthonormal basis $\{|i\rangle\}_{i=0}^{d-1}$ of the one-particle Hilbert space $\mathcal{H}_1^{(d)}$. The states

$$|i_1, i_2, \dots, i_N\rangle^{(f)} := \frac{1}{\sqrt{N!}} \sum_{\sigma \in S_N} \text{sign}(\sigma) |i_{\sigma^{-1}(1)}\rangle \otimes \dots \otimes |i_{\sigma^{-1}(N)}\rangle \quad (2.15)$$

will be called *Slater determinants*. They form an orthonormal basis of the fermionic Fock space $\mathcal{F}^{(f)}$. For the bosonic Fock space $\mathcal{F}^{(b)}$ one similarly defines orthonormal basis elements

$$|i_1, i_2, \dots, i_N\rangle^{(b)} := \frac{1}{\sqrt{N!}} \sum_{\sigma \in S_N} |i_{\sigma^{-1}(1)}\rangle \otimes \dots \otimes |i_{\sigma^{-1}(N)}\rangle \quad (2.16)$$

which will be called *permanents*.

At this point, let us introduce a convenient notational short form for Slater determinants that will become useful in later sections. Since the space $\mathcal{H}_N^{(f)}$ is spanned by $\binom{d}{N}$ Slater determinants that consist of N different single-particle states, we consider the set $\mathbb{P}_N^d$ of all N -subsets of $\{0, 1, \dots, d-1\}$:

$$\mathbb{P}_N^d := \left\{ X \subseteq \{0, 1, \dots, d-1\} \mid |X| = N \right\}. \quad (2.17)$$

Every N -tuple $\mathbf{s} = (s_1, \dots, s_N) \in \mathbb{P}_N^d$, which is called a configuration, defines a Slater determinant w.r.t. the orthonormal single-particle basis $\{|i\rangle\}_{i=0}^{d-1}$ via $|\mathbf{s}\rangle \equiv |s_1, \dots, s_N\rangle$. Consequently, the expansion of any N -fermion state $|\psi_N^{(f)}\rangle$ can be written as:

$$|\psi_N^{(f)}\rangle = \sum_{\mathbf{s} \in \mathbb{P}_N^d} c_{\mathbf{s}} |\mathbf{s}\rangle, \quad \forall c_{\mathbf{s}} \in \mathbb{C}. \quad (2.18)$$

The ladder operators $\hat{c}_{|\phi\rangle}$ and $\hat{c}_{|\phi\rangle}^\dagger$ create and annihilate fermions in the single-particle state $|\phi\rangle$. Their action onto arbitrary N -particle states can entirely be understood by considering the action of $\hat{c}_{|i\rangle}$ and $\hat{c}_{|i\rangle}^\dagger$ onto the Fock state basis (2.15) since $\hat{c}_{|\phi\rangle}$ can be written as a linear superposition of the $\hat{c}_{|i\rangle}$:

$$\begin{aligned}\hat{c}_{|i_1\rangle} |i_1, i_2, \dots, i_N\rangle^{(f)} &= |i_2, \dots, i_N\rangle^{(f)}, & \hat{c}_{|i_1\rangle}^\dagger |i_2, \dots, i_N\rangle^{(f)} &= |i_1, i_2, \dots, i_N\rangle^{(f)}, \\ \hat{c}_{|i_1\rangle} | \rangle &= 0.\end{aligned}\tag{2.19}$$

The vacuum state is represented by $| \rangle$. Evidently, the fermionic antisymmetry is equivalent to the following fermionic anti-commutation relations:

$$\{\hat{c}_{|i\rangle}, \hat{c}_{|j\rangle}^\dagger\} = \delta_{i,j}, \quad \{\hat{c}_{|i\rangle}, \hat{c}_{|j\rangle}\} = 0, \quad \{\hat{c}_{|i\rangle}^\dagger, \hat{c}_{|j\rangle}^\dagger\} = 0.\tag{2.20}$$

Henceforth, we shall abbreviate $\hat{c}_{|i\rangle}$ by $\hat{c}_i$ when the reference basis is known by context.

In the same manner, bosonic ladder operators $\hat{b}_{|\phi\rangle}$ and $\hat{b}_{|\phi\rangle}^\dagger$ can be defined by:

$$\begin{aligned}\hat{b}_{|i_1\rangle} |i_1, i_2, \dots, i_N\rangle^{(b)} &= \sqrt{n_{|i_1\rangle}} |i_2, \dots, i_N\rangle^{(b)}, \\ \hat{b}_{|i_1\rangle}^\dagger |i_2, \dots, i_N\rangle^{(b)} &= \sqrt{n_{|i_1\rangle} + 1} |i_1, i_2, \dots, i_N\rangle^{(b)}, & \hat{b}_{|i_1\rangle} | \rangle &= 0,\end{aligned}\tag{2.21}$$

where $n_{|i_1\rangle}$ represents the number of bosons in the one-particle state $|i_1\rangle$. The bosonic commutation relations read:

$$[\hat{b}_{|i\rangle}, \hat{b}_{|j\rangle}^\dagger] = \delta_{i,j}, \quad [\hat{b}_{|i\rangle}, \hat{b}_{|j\rangle}] = 0, \quad [\hat{b}_{|i\rangle}^\dagger, \hat{b}_{|j\rangle}^\dagger] = 0.\tag{2.22}$$

The ladder operators allow us to introduce another representation of the r -particle reduced density operator:

$$(\rho_r)_{i_1, \dots, i_r; k_1, \dots, k_r} \equiv \langle \mathbf{i} | \rho_r | \mathbf{k} \rangle := \left\langle \hat{a}_{i_1}^\dagger \dots \hat{a}_{i_r}^\dagger \hat{a}_{k_r} \dots \hat{a}_{k_1} \right\rangle_{\rho_N}.\tag{2.23}$$

The operators $\hat{a}_i$ and $\hat{a}_i^\dagger$ symbolise either fermionic or bosonic ladder operators. Note that by contrast to the earlier definition, this form of the reduced r -particle density operator is normalised to $\binom{N}{N-r}$. Commonly found in the literature of Quantum Chemistry, this convention especially implies that the 1-particle reduced density operator is normalised to the particle number. Unless stated otherwise, it will be adopted throughout the thesis.

Physical significance of ρ_1 and ρ_2

In (classical) Hamiltonians n -body terms depend on n -tuples $(\alpha_{i_1}, \dots, \alpha_{i_n}) \in \mathbb{K}^n$ of single-particle configuration space points. The n -body Hamiltonians associated with systems of indistinguishable particles are inherently invariant under particle exchanges. In the language of second quantisation they read:

$$\hat{H} = \hat{H}_0 + \sum_{m,m'} h_{mm'}^{(1)} \hat{a}_m^\dagger \hat{a}_{m'} + \sum_{m,l,m',l'} h_{mlm'l'}^{(2)} \hat{a}_m^\dagger \hat{a}_l^\dagger \hat{a}_{m'} \hat{a}_{l'} + \dots + \sum_{\dots} h_{\dots}^{(n)} \hat{a}_{m_1}^\dagger \dots \hat{a}_{m'_1} \dots + \dots \quad (2.24)$$

Again, $\hat{a}$ and $\hat{a}^\dagger$ can represent either bosonic or fermionic ladder operators. A detailed treatment of the second quantisation of n -body operators may be found in Ref. [76].

It is now a crucial observation that all physically relevant Hamiltonians only involve 1- and 2-body terms. By using Eq. (2.23) we can simplify the general expression of the energy functional:

$$E[\rho_N] := \text{tr}[\hat{H}\rho_N] \stackrel{(2.24)}{=} H_0 + \text{tr}[\hat{h}^{(1)}\rho_1] + \text{tr}[\hat{h}^{(2)}\rho_2] \equiv E[\rho_2], \quad (2.25)$$

where it is understood that $\rho_1 = \text{tr}_1[\rho_2]$. The energy functional becomes an effective functional of the 2-particle reduced density operator. Since the complexity of the many-particle Schrödinger equation grows exponentially with the number of particles, this reduction in complexity of the energy functional to $\mathcal{O}(d^4)$ has raised hopes to find a computationally more efficient description of many-body quantum systems in terms of reduced density operators [68, 97, 26, 24]. However, in order to carry out the variation of (2.25) w.r.t. ρ_2 , a set of (compact) constraints is required that guarantee the N -representability of the respective two-particle density operators.

Definition 1 (N -representability)

An r -particle density operator ρ_r is called pure-/ensemble- N -representable if it can be written as an r -particle reduced density operator of some pure/mixed N -particle density operator ρ_N : $\rho_r = \text{tr}_{N-r}[\rho_N]$. The problem of determining a compact form of the related set of necessary and sufficient conditions is generally known as the r -body pure-/ensemble- N -representability problem.³

More generally, the task of identifying a compact set of criteria on a tuple of density operators $\{\rho_A, \rho_B, \rho_C, \dots\}$ to form marginals of a multipartite quantum system is known as the *quantum marginal problem* [82]. A density operator ρ_A forms a *marginal*

³Unfortunately, the term of ‘ N -representability’ has seen ambiguous use in the literature. Whereas some authors (see, e.g., Ref. [63]) restrict its use to fermions, others include bosons, too (see, e.g., Ref. [19]). This thesis adopts the latter convention.

of the composite system $X = (A \cup B \cup \dots)$ if a density operator ρ_X exists, such that ρ_A is given by the partial trace of ρ_X : $\rho_A = \text{tr}_{X \setminus A}[\rho_X]$. Two marginals ρ_A and ρ_B are called *overlapping* if $A \cap B \neq \emptyset$. Accordingly, a quantum marginal problem is called overlapping if any two of the marginals overlap.

For $r \geq 2$ the r -body N -representability problem constitutes an example of an overlapping quantum marginal problem. Liu et al. [63] have proven the fermionic version to be QMA complete. Expressed in simplified terms this means that no tractable general solution can be derived.⁴ A similar result was shown to hold for bosons [104].

For $r = 1$ the problem becomes non-overlapping. The solution to a non-overlapping quantum marginal problem can be entirely expressed in terms of the spectra of the marginals and the total density operators. This is a consequence of local unitary equivalence: Given a tuple of marginals $\{\rho_A, \rho_B, \rho_C, \dots\}$ compatible with a composite state ρ_X , any tuple of marginals related by local unitaries, i.e. $\tilde{\rho}_A = \mathcal{U}_A \rho_A \mathcal{U}_A^\dagger$ etc., will be compatible with a composite state given by $\tilde{\rho}_X = (\mathcal{U}_A \otimes \dots) \rho_X (\mathcal{U}_A \otimes \dots)^\dagger$. In a series of ground-breaking works [1, 2, 50, 51, 52] Klyachko and Altunbulak derived the solution to the non-overlapping quantum marginal problem for pure and mixed states of the composite system. They found that the sets of compatible spectra are generally given by polytopes. In fermionic systems this has established the notion of Generalised Pauli constraints which are to be introduced subsequently. Before doing so and exploring the concept of reduced particle information more deeply in the next section, we shall add two closing remarks:

Firstly, as an immediate consequence of Eq. (2.1) we observe that systems with definite exchange symmetry will preserve this symmetry under unitary evolution.

Secondly, note that the anti-commutation relations (2.20) together with the positivity of the operators $\hat{c}_i \hat{c}_i^\dagger$ and $\hat{n}_i = \hat{c}_i^\dagger \hat{c}_i$ imply the famous Pauli exclusion principle:

$$0 \leq \langle \hat{n}_i \rangle \leq 1, \quad (2.26)$$

which can also be recasted as $0 \leq \rho_1 \leq 1$. In words: There can be no more than one fermion occupying the (arbitrary) single-particle state $|i\rangle$. Further also note that the inequalities (2.26) especially hold for the occupation numbers of the eigenstate basis. Since the largest and lowest eigenvalues of a hermitian operator constitute upper and lower boundaries on the occupation numbers of any arbitrary basis, one may regard

⁴In order to still make use of the simplified form of the energy functional (2.25) several techniques have been examined to provide an approximative description of the set of N -representable two-particle density matrices (see, e.g., Refs. [24, 38, 34, 108, 69]).

(2.26) as a constraint on the eigenvalues of $\rho_1^{(f)}$. For the remainder of this chapter, we will consider fermionic systems only and shall therefore omit the fermionic index on ladder and density operators.

2.3 Fermionic N -representability and Generalised Pauli Constraints

At the beginning of this section, two theorems on the 1-body N -representability of fermions will be presented. We shall consider settings with finite d -dimensional one-particle Hilbert spaces. Since we have a non-overlapping quantum marginal problem at hand, the solution can be expressed in terms of the spectra⁵ of the density operators (see related remarks in the previous section). This suggests the following useful definition:

Definition 2 (Natural occupation numbers and orbitals)

The eigenstates of the 1-particle (reduced) density operator are called natural orbitals and will be denoted by $\{|\phi_j\rangle\}_{j \in \mathcal{J}}$; the associated eigenvalues are called natural occupation numbers (NONs) λ_j . They form the non-increasingly ordered $\vec{\lambda}$ -vector of eigenvalues: $\vec{\lambda} \equiv (\lambda_j)_{j \in \mathcal{J}}^\downarrow$.

The Pauli exclusion principle (2.26) was shown to represent a necessary condition for the pure- and ensemble- N -representability of fermionic 1-RDOs. The following theorem ensures that it is also a *sufficient* condition for *ensemble- N -representability* (see, e.g., Ref. [24]):

Theorem 1 (Ensemble- N -representability)

A fermionic 1-particle density operator is ensemble- N -representable if and only if its normalised eigenvalues obey the Pauli exclusion principle:

$$0 \leq \lambda_j \leq 1, \quad \forall j \in \mathcal{J}; \quad \text{tr}[\rho_1] = \sum_{j \in \mathcal{J}} \lambda_j \equiv \|\vec{\lambda}\|_1 = N. \quad (2.27)$$

Proof: In order to show that (2.27) is not only necessary but also sufficient let us consider the *Pauli (hyper-) cube* $\mathcal{W}_d \equiv [0, 1]^d$ of all $\vec{\lambda} \in \mathbb{R}^d$ obeying the exclusion principle. The extremal points of this linearly closed and linearly bounded convex set are given by the 2^d different vectors with entries 0 or 1. The convex subset $\bar{\mathcal{W}}_d$ of N -normalised vectors within the Pauli cube is yielded by intersection of $\mathcal{W}_d$ with

⁵In the case of finite dimensional Hilbert spaces the spectrum coincides with the set of eigenvalues.

the hyperplane defined by $\text{tr}[\rho_1] = N$. Due to the theorem of Dubins,⁶ the extremal points of $\bar{\mathcal{W}}_d$ are given by the $\binom{d}{N}$ vectors $\vec{s}_i$ with N entries 1 and $d - N$ entries 0. Consequently, some arbitrary vector $\vec{\lambda}$ fulfilling (2.27) can be written as a convex combination of the vectors $\vec{s}_i$: $\vec{\lambda} = \sum_i q_i \vec{s}_i$, where $q_i \geq 0$. One may now construct Slater determinants $|\mathbf{s}_i\rangle$ of the single-particle natural orbitals corresponding to the occupations indicated by each $\vec{s}_i$. The ensemble N -particle state derived by convex superposition $\rho_N = \sum_i q_i |\mathbf{s}_i\rangle \langle \mathbf{s}_i|$ then constitutes an N -representation of the 1-body state defined by $\vec{\lambda}$.

Generalised Pauli Constraints

Unlike the ensemble- N -representability problem, the pure 1-body- N -representability problem turns out to be much more intricate. For a long time after Pauli's work [75] it was unknown whether the conditions (2.27) would also be sufficient to guarantee N -representability by a pure state. First evidence that further constraints would be required in at least some cases was found by Borland and Dennis in 1970 [12]. The generalisation to arbitrary numbers of particles N and single-particle states d was eventually derived in the remarkable works by Klyachko and Altunbulak (see Refs. [1, 2, 50, 51, 52]). Their results may (without proof) be summarised in the following theorem:

Theorem 2 (Pure N -representability and Generalised Pauli Constraints)

For arbitrary but fixed N and d , the set of fermionic 1-particle density operators that are representable by a pure N -particle state is determined by a finite set of linear constraints on the N -normalised $\vec{\lambda}$ -vector associated with ρ_1 :

$$D_j(\vec{\lambda}) = \kappa_j^{(0)} + \sum_{i=1}^d \kappa_j^{(i)} \cdot \lambda_i = \kappa_j^{(0)} + \vec{\kappa}_j \cdot \vec{\lambda} \geq 0 \quad \text{for } j \in 1 \dots r_{N,d}, \quad \|\vec{\lambda}\|_1 = N. \quad (2.28)$$

The number of constraints $r_{N,d}$ is finite. It is further a non-trivial mathematical fact that all coefficients $\kappa_j^{(0)}$ and $\kappa_j^{(i)}$ can be chosen as integers. The inequalities (2.28) are called Generalised Pauli Constraints (GPCs) of the setting $\wedge^N[\mathcal{H}_1^{(d)}]$. The set of all functions D_j will be denoted by $\mathcal{G}_{N,d}$.

The relation between the GPCs and the Pauli exclusion principle is best understood by a geometrical illustration of the constraints. Each GPC in (2.28) describes a half-space of allowed $\vec{\lambda}$ -vectors in $\mathbb{R}^d$. The intersection of all these half-spaces forms

⁶“Every extreme point of a convex set derived by intersection of a linearly bounded and linearly closed convex set C with m hyperplanes is a convex combination of at most $m + 1$ extreme points of C .” Cf. Ref. [32].

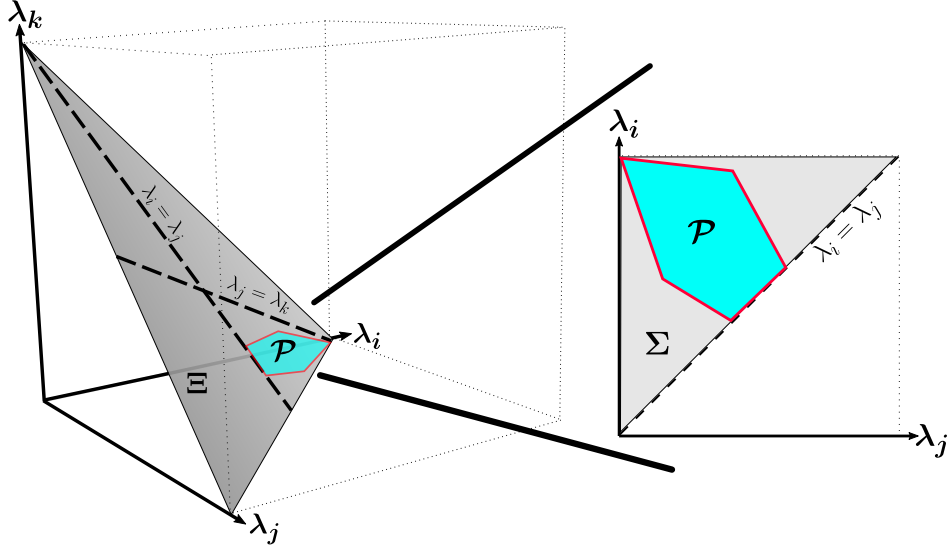


Figure 2.1: Schematic illustration of the GPC-polytope geometry. Left: Hyperplane Ξ of normalised vectors within the $(\lambda_i, \lambda_j, \lambda_k)$ -subspace of the Pauli hyper-cube $\mathcal{W}_d$ (dotted box frame). The ordering constraints $\lambda_i \geq \lambda_j$ and $\lambda_j \geq \lambda_k$ are marked with dashed lines. The polytope $\mathcal{P}$ results from further intersection with halfspaces defined by the GPCs. The schematic boundary of the polytope is marked by red segments. Right: Reduction of the illustration to the (λ_i, λ_j) -subspace. Note that the polytope $\mathcal{P}$ is a proper subset of the Pauli simplex Σ .

a polytope within the Pauli hypercube $\mathcal{W}_d$. Additionally, one has to take into account the normalisation condition and the ordering constraints $\lambda_i \geq \lambda_{i+1}$, which also correspond to half-spaces. The resulting set becomes a polytope again:

$$\mathcal{P}^{(N,d)} := \{\vec{\lambda} \in \mathbb{R}^d | D_j(\vec{\lambda}) \geq 0, \forall j = 1 \dots r_{N,d}, \wedge \lambda_i \geq \lambda_{i+1} \wedge \|\vec{\lambda}\|_1 = N\}. \quad (2.29)$$

This polytope is contained within the *Pauli simplex*, which consists of all non-increasingly ordered vectors fulfilling the conditions (2.27):

$$\Sigma^{(N,d)} := \{\vec{\lambda} \in \mathbb{R}^d | 0 \leq \lambda_i \leq 1, \forall j = 1 \dots d, \wedge \lambda_i \geq \lambda_{i+1} \wedge \|\vec{\lambda}\|_1 = N\}. \quad (2.30)$$

Note that $\mathcal{P}^{(N,d)} \subsetneq \Sigma^{(N,d)}$ directly implies that the Pauli exclusion principle is a weaker constraint on pure states than the antisymmetry of the N -fermionic wave function. A sketch of these geometrical concepts is shown in Fig. 2.1 where a section of the λ -space is displayed. It is a crucial observation that some half-space can *ab initio* not be related to an inequality with unique coefficients since each common multiple of the coefficients would give rise to the same set of points. This induces an ambiguity in the representation of the GPCs in form of D_j functions. However, the non-trivial fact that all coefficients may be chosen to be integers allows one to define

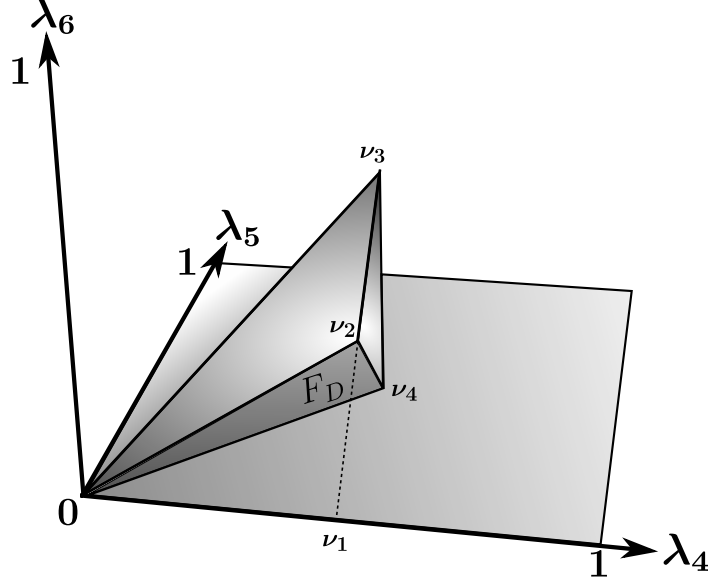


Figure 2.2: $(\lambda_4, \lambda_5, \lambda_6)$ -space of the Borland-Dennis polytope. The extremal points read $\nu_2 = (\frac{1}{2}, \frac{1}{4}, \frac{1}{4})$, $\nu_3 = (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$, $\nu_4 = (\frac{1}{2}, \frac{1}{2}, 0)$ and $\mathbf{0} = (0, 0, 0)$. The facets $\overline{\mathbf{0}\nu_2\nu_3}$, $\overline{\mathbf{0}\nu_3\nu_4}$ and $\overline{\nu_2\nu_3\nu_4}$ correspond to the ordering constraints $\lambda_5 \geq \lambda_6$, $\lambda_4 \geq \lambda_5$ and $\lambda_3 \geq \lambda_4$, respectively. The inequality constraint (2.31b) specifies the facet $\overline{\mathbf{0}\nu_2\nu_4}$ tagged by F_D . The Pauli simplex $\Sigma^{(3,6)}$ is given by $\overline{\mathbf{0}\nu_1\nu_4\nu_3}$, where $\nu_1 = (\frac{1}{2}, 0, 0)$.

a unique representation of the constraints by requiring the $\kappa_j^{(i)}$ to assume the smallest possible integer values.

Let us now briefly discuss the Borland-Dennis setting [12] as an important example of GPCs. The GPCs of the setting $\wedge^3[\mathcal{H}_1^{(6)}]$ are given by:

$$\lambda_1 + \lambda_6 = \lambda_2 + \lambda_5 = \lambda_3 + \lambda_4 = 1, \quad (2.31a)$$

$$\lambda_1 + \lambda_2 + \lambda_4 \leq 2. \quad (2.31b)$$

Due to the three equalities (2.31a), the set of compatible $\vec{\lambda}$ -vectors can be displayed in the $(\lambda_4, \lambda_5, \lambda_6)$ -space, cf. Fig. 2.2. By this means, all (full six-dimensional) $\vec{\lambda}$ -vectors are automatically normalised. The inequality gives rise to the facet of the polytope spanned by the points $(0, 0, 0)$, ν_2 and ν_4 and indicated by F_D . The other facets originate from the ordering constraints (see figure capture). The Pauli simplex $\Sigma^{(3,6)}$ is spanned by the points $(0, 0, 0)$, ν_1 , ν_3 and ν_4 and thus satisfies the embedding relation $\mathcal{P}^{(3,6)} \subsetneq \Sigma^{(3,6)}$.

A couple of other settings of GPCs are provided in the appendix, Sec. A. In principle, all settings of GPCs may be computed with help of the algorithm invented by Altunbulak and Klyachko (see, e.g., Ref. [2]). Unfortunately, the computational

resources required by this algorithm increase severely with the number of particles N and dimensions d . So far, the GPCs are known for settings of up to $N = 5$ particles in $d = 10$ dimensions and $N = 3$ particles in $d = 11$ dimensions. An alternative approach to the computation of GPCs was suggested by Bürgisser et al. in 2015 [15] (also cf. Ref. [21]). However, the description of higher-dimensional GPCs still remains to be an open question. As we shall see further below, this poses a major challenge to all physical applications since the required active spaces typically have dimensions much larger than $d = 10$. Additional structural insight into the GPCs is given by the particle-hole duality and a type of consistency requirement between settings of different dimensions and particle numbers.

Particle-hole duality and the inclusion relation for GPCs

The particle-hole duality has its origin in a natural isomorphism between the N -fermion and the $(d - N)$ -fermion Hilbert spaces: $\wedge^N[\mathcal{H}_1^{(d)}] \simeq \wedge^{(d-N)}[\mathcal{H}_1^{(d)}]$. This isomorphism establishes a one-to-one correspondence between the two respective sets of N -representable $\vec{\lambda}$ -vectors. Every GPC of the (N, d) setting gives rise to a GPC of the $(d - N, d)$ -setting:

$$D_j^{(d-N, d)}(\lambda_1, \lambda_2, \dots, \lambda_d) := D_j^{(N, d)}(1 - \lambda_d, 1 - \lambda_{d-1}, \dots, 1 - \lambda_1), \quad \forall j \in 1 \dots r_{N, d}. \quad (2.32)$$

Another important property of GPCs linking settings of higher particle numbers and dimensions to smaller settings is given by the *inclusion relation*. By physical intuition one might surmise that a simplified description of an N -fermion system, in which certain orbitals will remain occupied by ‘frozen’ fermions, while other orbitals will remain unoccupied, can be provided by considering the ‘active’ levels only. ‘Active levels’ in this context refers to those natural orbitals whose associated natural occupation numbers are strictly smaller than one and larger than zero. For pure states this idea can be given a precise formulation in terms of GPCs as follows: A $\vec{\lambda}$ -vector with u entries 1 and v entries 0 is compatible with a pure state of the $\wedge^{u+N}[\mathcal{H}_1^{(d+u+v)}]$ -setting if the reduced $\vec{\lambda}$ -vector, consisting of the d active occupation numbers, is compatible with a pure state of the smaller setting $\wedge^N[\mathcal{H}_1^{(d)}]$.

$$\begin{aligned} \vec{\lambda} \equiv (\underbrace{1, \dots, 1}_u, \lambda_1, \lambda_2, \dots, \lambda_d, \underbrace{0, \dots, 0}_v) &\in \mathcal{P}^{(u+N, d+u+v)} \\ \text{if and only if } \vec{\lambda}^{(r)} \equiv (\lambda_1, \lambda_2, \dots, \lambda_d) &\in \mathcal{P}^{(N, d)}. \end{aligned} \quad (2.33)$$

Geometrically, this can be regarded as an isomorphism between the projected polytope $\mathcal{P}^{(u+N, d+u+v)}$ and $\mathcal{P}^{(N, d)}$:

$$\mathcal{P}^{(N+u, d+u+v)} \Big|_{\substack{\lambda_{d+u+1}=\dots=\lambda_{d+u+v}=0 \\ \lambda_1=\dots=\lambda_u=1}} \simeq \mathcal{P}^{(N, d)}. \quad (2.34)$$

For a proof we refer to Ref. [84].

Finally, it shall be remarked that the inclusion relation in the form of (2.33) or (2.34) does *not* induce a one-to-one correspondence between the sets $\mathcal{G}_{N+u,d+u+v}$ and $\mathcal{G}_{N,d}$. However, it is ensured that for every GPC of the smaller setting there will be a GPC of the larger setting whose projection yields the smaller one:

$$\mathcal{G}_{N,d} \ni D'_j \quad : \quad \exists D_j \in \mathcal{G}_{N+u,d+u+v}, \quad (2.35)$$

such that $D'_j(\lambda_1, \lambda_2, \dots, \lambda_d) = D_j(\underbrace{1, \dots, 1}_u, \lambda_1, \lambda_2, \dots, \lambda_d, \underbrace{0, \dots, 0}_v)$.

2.4 (Quasi-)pinning of GPCs

The remarkable discovery of the GPCs raises the question about their physical significance. Among other potential physical manifestations, the *pinning effect* postulated by Klyachko [52, 53] presents the perhaps most exceptional one. Klyachko proposed that under minimisation of the energy functional $\langle \psi_N | \hat{H} | \psi_N \rangle$ the system might assume a ground state whose NONs saturated some GPCs. Any further reduction of $\langle \psi_N | \hat{H} | \psi_N \rangle$ would require a violation of the GPCs which was prohibited by the fundamental nature of fermions. Therefore, the $\vec{\lambda}$ -vector would be pinned to the boundary of the polytope $\mathcal{P}$.

In his PhD thesis [84], Schilling raised the objection that since $\langle \psi_N | \hat{H} | \psi_N \rangle$ was a functional of the 2-RDO, the minimisation would certainly lead to “pinning” on the level of 2-RDOs, but that the same could not generally be expected for the 1-RDO. It thus comes as a surprise that in various systems the $\vec{\lambda}$ -vector can be found very close to, but not exactly on the polytope boundary. This effect was coined as *quasipinning* and shall be made precise with the following definition (cf. Ref. [87, 84]):

Definition 3 (Pinning and Quasipinning)

If the distance between the $\vec{\lambda}$ -vector of a pure N -fermion quantum state and the boundary of the polytope $\partial\mathcal{P}$ is comparatively small to the extent of the Pauli hypercube:

$$\text{dist}(\vec{\lambda}, \partial\mathcal{P}) \ll 1, \quad (2.36)$$

then the system is said to exhibit quasipinning. If the $\vec{\lambda}$ -vector lies exactly on $\partial\mathcal{P}$, i.e. if $\text{dist}(\vec{\lambda}, \partial\mathcal{P}) = 0$, then this shall be called pinning.

Note that the unit length of the Pauli hypercube constitutes a natural length scale in the space of NONs.

In order to understand why *quasipinning* should be physically relevant one has to specify the distance measure used in Def. 3. Before doing so, an extraordinary structural property of pinned N -fermion states shall be discussed. Let us denote the ladder operators for the natural orbital basis $\{|\phi_j\rangle\}_{j \in \mathcal{J}}$ of some N -fermion state $|\psi_N\rangle$ with corresponding NONs $\vec{\lambda}$ by $\hat{a}_j$ and $\hat{a}_j^\dagger$. For a GPC $D \in \mathcal{G}_{N,d}$ (2.28) with coefficients κ_0 and $\vec{\kappa}$ define the operator:

$$\hat{D}_{|\psi_N\rangle} := \kappa_0 \mathbb{1} + \kappa_1 \hat{a}_1^\dagger \hat{a}_1 + \dots + \kappa_d \hat{a}_d^\dagger \hat{a}_d. \quad (2.37)$$

Obviously, we have $D(\vec{\lambda}) = \langle \psi_N | \hat{D}_{|\psi_N\rangle} | \psi_N \rangle$ which implies

$$D(\vec{\lambda}) = 0 \quad \Longleftrightarrow \quad \langle \psi_N | \hat{D}_{|\psi_N\rangle} | \psi_N \rangle = 0. \quad (2.38)$$

Furthermore, a theorem can be proven [64] that establishes even a stronger relation:

$$D(\vec{\lambda}) = 0 \quad \Longrightarrow \quad \hat{D}_{|\psi_N\rangle} | \psi_N \rangle = 0. \quad (2.39)$$

Note that this is quite unexpected since $\hat{D}_{|\psi_N\rangle}$ has positive *and* negative eigenvalues. As a consequence, the pinning of a GPC D by a $\vec{\lambda}$ -vector associated with $|\psi_N\rangle$ imposes a selection rule on the expansion series coefficients of $|\psi_N\rangle$:

Corollary 1 (Selection rule on Slater determinants)

Let $|\psi_N\rangle = \sum_{\mathbf{k} \in \mathbb{P}_N^d} c_{\mathbf{k}} |\mathbf{k}\rangle$ be the self-consistent expansion of the N -fermion state $|\psi_N\rangle$ in terms of Slater determinants of its natural orbitals. Further assume that the associated $\vec{\lambda}$ -vector of $|\psi_N\rangle$ saturates the GPC D , i.e. $D(\vec{\lambda}) = 0$. Then Eq. (2.39) implies that:

$$\hat{D} |\mathbf{k}\rangle \neq 0 \quad \Longrightarrow \quad c_{\mathbf{k}} = 0. \quad (2.40)$$

One recognises that the number of Slater determinants required in an expansion of the N -fermion state is significantly reduced if the corresponding $\vec{\lambda}$ -vector is pinned to the boundary of the polytope.

To illustrate this remarkable property of the GPCs, let us examine the selection rule emerging from the Borland-Dennis setting (2.31). By the equality constraints (2.31a), the number of Slater determinants required for an expansion of some arbitrary state $|\psi_N\rangle$ is reduced to 8. If the inequality constraint (2.31b) is saturated, then the corresponding 3-fermion state can be simplified further:

$$|\psi_{BD}\rangle = a |1, 2, 3\rangle + b |1, 4, 5\rangle + c |2, 4, 6\rangle. \quad (2.41)$$

Here, the Slater determinants are defined with respect to the natural orbitals of $|\psi_{BD}\rangle$.

Let us stress the significance of the selection rule. By extremising the one-particle information, one obtains additional structural insight about the N -particle information.

In his thesis [84], Schilling conjectured that the selection rule (2.40) could be extended to quasipinned states. More specifically, for an N -fermion state $|\psi_N\rangle$ with associated NONs $\vec{\lambda}$ and $D(\vec{\lambda}) = \delta \ll 1$, the L^2 -weight of $|\psi_N\rangle$ on the subspace of Slater determinants suppressed by Eq. (2.40) is of the order $\mathcal{O}(\delta)$.

$$1 - |\langle \psi_N | P_D | \psi_N \rangle|^2 \leq \mathcal{O}(\delta). \quad (2.42)$$

Here, P_D denotes the projector onto the subspace of Slater determinants selected by Eq. (2.40). Only recently, a proof of this conjecture was found [81] and is going to be published soon.

Note that Eq. (2.42) may be regarded as a generalisation of the single-Slater determinant approximation of weakly correlated systems. If the particle-particle interactions are comparatively weak, the $\vec{\lambda}$ -vector will be found close to the Hartree-Fock point $\vec{\lambda}_{HF}$:

$$\vec{\lambda}_{HF} = \{\underbrace{1, \dots, 1}_N, \underbrace{0, \dots, 0}_{d-N}\}. \quad (2.43)$$

The deviation of the $\vec{\lambda}$ -vector from this point sets bounds on the overlap of the weakly correlated N -fermion state with a single Slater determinant.

Let us return to the question of quantifying the strength of quasipinning by specifying the distance measure in Def. 3. Due to the significance of the selection rule in corollary 1, one may propose the following measure:

$$D_{min}(\vec{\lambda}) := \min_j D_j(\vec{\lambda}). \quad (2.44)$$

Indeed, it can be shown that for $D_{min}(\vec{\lambda}) \ll 1$, the measure D_{min} reproduces the geometrical l_1 distance between the $\vec{\lambda}$ -vector and the boundary of the polytope⁷ up to a prefactor:

$$dist_1(\vec{\lambda}, \partial\mathcal{P}) = \min_j \left(\frac{2D_j(\vec{\lambda})}{\Delta\kappa_{j,max}} \right) \propto D_{min}(\vec{\lambda}), \quad (2.45)$$

where $\Delta\kappa_{j,max} := \max_{k,l>0} \{|\kappa_j^{(k)} - \kappa_j^{(l)}|\}$. A proof may be found in Ref. [94]. For other l_p distance measures the dependence of $dist_p(\vec{\lambda}, \mathcal{P})$ on D_{min} becomes more involved.

⁷Note that here $\partial\mathcal{P}$ does not strictly refer to the entire polytope boundary but rather only encompasses the facets defined by the respective GPCs.

Therefore, the measure D_{min} is the most natural choice and shall thus be used to quantify quasipinning throughout the rest of this thesis.⁸ Generally, quasipinning shall be said to become “stronger” when D_{min} decreases.

Pinning analysis and method of truncation

In order to use the minimal distance measure D_{min} for the evaluation of quasipinning in physical systems, it is necessary to provide practical means of its computation for a given set of NONs. For systems with a finite dimensional one-particle Hilbert space, the procedure is apparently simple: By evaluating the finite set of GPCs at the finite dimensional $\vec{\lambda}$ -vector and taking the minimum of all outcomes, one can determine the minimal distance D_{min} . However, a major obstacle to this is given by the fact that the form of the GPCs is only known for a limited number of smaller settings $\wedge^N[\mathcal{H}_1^{(d)}]$ (cf. discussion in the previous section). The situation becomes even more difficult if one considers physical systems with *infinite* dimensional one-particle Hilbert spaces.

As a consequence, many works (cf., e.g., Refs. [52, 7, 18, 9, 96]) have resorted to truncating the one-particle Hilbert space *before* solving the Schrödinger equation. With this approach to a pinning analysis, however, one encounters the unfortunate side-effect of having no knowledge or control on the truncation induced error in the quasipinning measure.

A method to overcome this difficulty is given by the concept of a so-called *truncated pinning analysis* [84, 93]. The idea of this technique is to derive a sufficiently accurate set of NONs *before* truncating the $\vec{\lambda}$ -vector. Let $|\psi_{N'}\rangle$ be an N' -fermion state in $\wedge^{N'}[\mathcal{H}_1^{d'}]$ with exact $\vec{\lambda}$ -vector $\vec{\lambda}' = \{\lambda'_i\}_{i=1}^{d'}$. Due to the inclusion relation into the reduced setting $\wedge^N[\mathcal{H}_1^d]$ with $N' \geq N$ and $d' \geq d$ (see Eqs. (2.33) and (2.35)), we find that every GPC $D'_j \in \mathcal{G}_{N',d'}$ can be assigned to one of the following two cases:

1. In the reduced setting of $\wedge^N[\mathcal{H}_1^d]$ there exists a GPC D_j , such that:

$$D_j(\vec{\lambda}^{(r)}) = D'_j(\underbrace{1, \dots, 1}_{N'-N}, \vec{\lambda}^{(r)}, \underbrace{0, \dots, 0}_{d'-d-N'+N}), \quad \forall \vec{\lambda}^{(r)} \in \mathcal{P}^{(N,d)}. \quad (2.46)$$

2. For all $\vec{\lambda}^{(r)} \in \mathcal{P}^{(N,d)}$, the inequality $D'_j(1, \dots, 1, \vec{\lambda}^{(r)}, 0, \dots, 0) \geq 0$ is either implied by a set of inequalities $D_j(\vec{\lambda}^{(r)}) \geq 0$ or becomes a simple tautology: $D'_j(1, \dots, 1, \vec{\lambda}^{(r)}, 0, \dots, 0) = \text{const.} \geq 0$.

⁸Note that the global measure of the minimal distance D_{min} (2.44) can further be refined by considering the set of minimal distances to all GPC facets $F_{D_j} := \{\vec{\lambda} \in \mathcal{P} \mid D_j(\vec{\lambda}) = 0\}$.

Due to the linearity of the GPCs, one can thus estimate the true minimal distance of $\vec{\lambda}'$ to the boundary of $\mathcal{P}^{(N',d')}$:

$$D'_j(\vec{\lambda}') = D_j(\vec{\lambda}^{(r)}) + \mathcal{O}(1 - \lambda'_{N'-N}) + \mathcal{O}(\lambda'_{d+N'-N+1}). \quad (2.47)$$

In summary, the concept of the truncated (quasi-)pinning analysis consists of the following steps:

1. Derivation of the exact (or sufficiently accurate) NONs $\vec{\lambda}'$ of the N' -fermion state $|\psi_{N'}\rangle \in \wedge^{N'}[\mathcal{H}_1^{d'}]$ to be investigated.
2. Truncation of the $\vec{\lambda}'$ -vector to a d -dimensional vector $\vec{\lambda}^{(r)}$.
3. Evaluation of the minimal distance of $\vec{\lambda}^{(r)}$ to the boundary of the reduced polytope $\mathcal{P}^{(N,d)}$.
4. If the outcome is larger than the truncation error, then the analysis has been conclusive. Otherwise it becomes necessary to choose a larger-dimensional truncated $\vec{\lambda}$ -vector. From Eq. (2.47) we see that this error is of the order $\max[\mathcal{O}(1 - \lambda'_{N'-N}), \mathcal{O}(\lambda'_{d+N'-N+1})]$

In the following chapter, the truncated quasipinning analysis will be applied to various systems. An explicit example of its step-by-step implementation will be provided in Sec. 3.3.1.

Further note that the structure of the truncated (quasi-)pinning analysis also supports the choice of D_{min} (i.e. l_1) as the quasipinning measure. If a different norm l_p , $p > 1$ was used, the more involved dependence of $dist_p(\cdot, \cdot)$ on $D(\cdot)$ would imply that adding “frozen” fermions and unoccupied levels changed the quasipinning of the system. Therefore, the minimal distance measure D_{min} (2.44) and with it the l_1 distance provide the most natural choice.

In the final section of this chapter we are now going to examine the relevance of the GPCs beyond the well-known Pauli exclusion principle.

2.5 The Q -parameter

In the previous section we have seen that the values $\{D_j(\vec{\lambda})\}$ provide an *absolute* measure of the quasipinning strength. It was further outlined that strong quasipinning is an indicator for a crucial role of the fermionic antisymmetry in the behaviour of the system. Yet, as we shall now elaborate, such influence can sometimes already

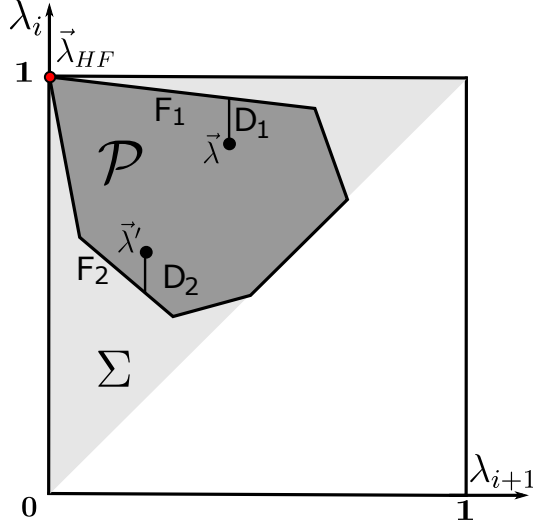


Figure 2.3: Minimal l_1 -distances $D_{min} = D_1, D_2$ of two different vectors $\vec{\lambda}$ and $\vec{\lambda}'$ to the polytope facets F_1 and F_2 . The polytope $\mathcal{P}$ is a proper subset of the Pauli simplex Σ , the Hartree-Fock point (2.43) is marked by a red point (see Eq. (2.44) and text for more details).

be expected from the approximate saturation of the weaker Pauli exclusion principle constraints (2.26). In particular, the question arises: What additional physical insights can be gained by incorporating the GPCs into the description of fermionic systems? In order to answer this question, one has to quantify the amount by which the quasipinning of GPCs is already implied by the quasipinning of the respective Pauli exclusion principle constraints.

Let us start by considering the schematical drawing of the polytope $\mathcal{P}$ and the Pauli simplex Σ in Fig. 2.3. Since the polytope $\mathcal{P}$ (2.29) is a proper subset of the Pauli simplex Σ (2.30) one recognises that $\vec{\lambda}$ -vectors close to the boundary of Σ must also lie close to the boundary of the polytope. Observe that the quasipinning of the NONs $\vec{\lambda}$ to the Pauli exclusion principle constraint $\lambda_i \leq 1$ also corresponds to an approximate saturation of the GPC D_1 . However, the quasipinning of the NONs $\vec{\lambda}'$ to the facet F_2 can *not* be inferred from approximate quasipinning of any Pauli exclusion principle constraint.

For instance, consider the GPC $D_{12}^{(4,8)}$ of the setting $\wedge^4[\mathcal{H}_1^{(8)}]$ (see, e.g., Eq. (A.2)):

$$D_{12}^{(4,8)}(\vec{\lambda}) := 2 - \lambda_1 - \lambda_4 - \lambda_5 + \lambda_8 \geq 0. \quad (2.48)$$

For all NONs that saturate the Pauli exclusion constraints $\lambda_1 \leq 1$ and $\lambda_8 \geq 0$, this GPC reduces to $1 - \lambda_4 - \lambda_5 \geq 0$. By invoking the inclusion relation (2.33) one finds that this inequality is equivalent to the inequality $1 - \lambda'_3 - \lambda'_4 \geq 0$ in the reduced setting

$\wedge^3[\mathcal{H}_1^{(6)}]$, which is the Borland-Dennis setting (2.31). Notice that, due to its equality constraints (2.31a), the reduced inequality of the GPC $D_{12}^{(4,8)}$ will be automatically saturated. Therefore, $D_{12}^{(4,8)}$ is exactly pinned whenever λ_1 and λ_8 are pinned by the Pauli exclusion principle.

In the following, these ideas shall be formally worked out. By a geometrical analysis of the GPCs, we find them to be hierarchically ordered in different classes. This and a proper definition of the Pauli simplex facets will pave the way for the definition of a measure Q , which will evaluate the relevance of the GPCs *beyond* the exclusion principle.

Recall that the polytope $\mathcal{P}$ is a proper subset of the Pauli simplex Σ . This implies that for all $\vec{\lambda} \in \mathcal{P}$ we have $\vec{\lambda} \in \partial\Sigma \Rightarrow \vec{\lambda} \in \partial\mathcal{P}$. Note that the boundaries of $\mathcal{P}$ and Σ also comprise the facets defined by the ordering constraints $\lambda_i \geq \lambda_{i+1}$. In order to explore the geometric relation between proper constraint facets of the GPCs and the exclusion principle, introduce the functions S and respective inequalities

$$S_{r,s}(\vec{\lambda}) := \sum_{i=1}^r (1 - \lambda_i) + \sum_{k=d+1-s}^d \lambda_k \geq 0, \quad (2.49)$$

which are equivalent to the Pauli exclusion principle constraints (2.26). Here, $r \leq N$, $s \leq d - N$ and $r + s > 0$. These constraints give rise to the facets of the Pauli simplex:

$$\begin{aligned} \Sigma_{r,s} &:= \{ \vec{\lambda} \in \Sigma \mid S_{r,s}(\vec{\lambda}) = 0 \} \\ &= \Sigma \Big|_{\substack{\lambda_1 = \dots = \lambda_r = 1 \\ \lambda_{d+1-s} = \dots = \lambda_d = 0}}. \end{aligned} \quad (2.50)$$

The Pauli simplex facet $\Sigma_{r,s}$ corresponds to all $\vec{\lambda}$ -vectors of the Pauli simplex, which have r entries 1 and s entries 0. Obviously, $\Sigma_{N,d-N}$ is given by the Hartree-Fock point (2.43) and contained within the next larger facet $\Sigma_{N-1,d-N-2}$. More generally, the following nesting relation holds:

$$\Sigma_{r,s} \subseteq \Sigma_{r',s'} \quad \text{if and only if} \quad r \geq r' \text{ and } s \geq s'. \quad (2.51)$$

As an example, consider Pauli-simplex facets of the Borland-Dennis setting in Fig. 2.2. The facet $\Sigma_{3,3}$ is given by the point $\mathbf{0}$, the facet $\Sigma_{2,2}$ by the line $\overline{\mathbf{0}\nu_1}$ and the facet $\Sigma_{1,1}$ by the triangle $\overline{\mathbf{0}\nu_1\nu_4}$.

Let us define the facet F_j of a GPC D_j :

$$F_j := \{ \vec{\lambda} \in \mathcal{P} \mid D_j(\vec{\lambda}) = 0 \}. \quad (2.52)$$

For an arbitrary but fixed pair of indices (r, s) , the saturation of the constraint $S_{r,s} \geq 0$ implies pinning of the GPC D_j if and only if

$$F_j \supset \mathcal{P} \cap \Sigma_{r,s} \simeq \mathcal{P}', \quad (2.53)$$

where due to the inclusion relation (2.33) the polytope $\mathcal{P}'$ is associated with the setting $\wedge^{(N-r)}[\mathcal{H}_1^{(d-r-s)}]$. Explicitly written out, Eq. (2.53) reads

$$D_j(\underbrace{1, \dots, 1}_r, \vec{\lambda}', \underbrace{0, \dots, 0}_s) = 0, \quad \forall \vec{\lambda}' \in \mathcal{P}'. \quad (2.54)$$

Note that this recovers the approach in our example (2.48) above.

The relation (2.53) allows us to define the natural classes $\mathcal{C}_{r,s}$ of GPCs:

$$\mathcal{C}_{r,s} := \{D_j \in \mathcal{G}_{N,d} \mid \mathcal{P} \cap \Sigma_{r,s} \supset F_j\}. \quad (2.55)$$

The class $\mathcal{C}_{r,s}$ contains all those GPCs which are automatically pinned for all $\vec{\lambda}$ -vectors with r entries 1 and s entries 0. The hierarchy of Pauli simplex facets (2.51) is inherited by the classes $\mathcal{C}_{r,s}$:

$$\mathcal{C}_{r,s} \subseteq \mathcal{C}_{r',s'} \quad \text{if and only if} \quad r \leq r' \text{ and } s \leq s'. \quad (2.56)$$

This imposes a partial ordering on the set of index pairs (r, s) . Consequently, for each GPC D_j whose facet contains the Hartree-Fock point, there exists a minimal pair (r, s) .⁹ Practically, this pair can be determined by extremising the projected constraint (2.54) over the domain of the reduced polytope $\mathcal{P}'$. For each fixed trial pair (r, s) , this task can be accomplished by a linear algorithm (see appendix, Sec. D for an introduction to constrained optimisation). The corresponding results are displayed in the tables of the appendix, Sec. A. Let us emphasise that the minimal pair (r, s) of a GPC D_j states the minimal numbers of 1's and 0's one has to substitute into $\vec{\lambda}$, such that $D_j(\vec{\lambda})$ will be *automatically* pinned.

We have seen that the pinning of some Pauli exclusion principle constraint $S_{r,s}$ (2.49) implies pinning of all GPCs contained within the class $\mathcal{C}_{r,s}$. Obviously, this also extends to quasipinning. Recall that the l_1 distance of $\vec{\lambda}$ to the facet F_j of a GPC D_j is a *linear* function in the NONs (see Eq. (2.45)). A similar relation can be derived for the l_1 distance of $\vec{\lambda}$ to the Pauli simplex facet $\Sigma_{r,s}$:

$$\text{dist}_1(\vec{\lambda}, \Sigma_{r,s}) = S_{r,s}(\vec{\lambda}). \quad (2.57)$$

⁹If for some GPC D_j one has $D_j(\vec{\lambda}_{HF}) > 0$, then the facet does not intersect the Hartree-Fock point and no minimal pair exists. This corresponds to the facet F_2 in Fig. 2.3.

Therefore, we find that $dist_1(\vec{\lambda}, F_j)$ is *linearly* bounded from above by $dist_1(\vec{\lambda}, \Sigma_{r,s})$:

$$dist_1(\vec{\lambda}, F_j) \leq c_j dist_1(\vec{\lambda}, \Sigma_{r,s}), \quad (2.58)$$

for all pairs (r, s) with $D_j \in \mathcal{C}_{r,s}$, of which henceforth, due to the nesting relation (2.51), the minimal pair shall be chosen. The prefactor c_j is given by

$$c_j := \min_{\vec{\lambda} \in \mathcal{P}} \left(\frac{dist_1(\vec{\lambda}, \Sigma_{r,s})}{dist_1(\vec{\lambda}, F_j)} \right). \quad (2.59)$$

For any pair (r, s) and GPC D_j , c_j can be derived by means of a constrained optimisation. Example results are included in the tables of the Appendix A. Note that the inequality (2.58) can also be regarded as an immediate consequence of the flat geometry of the polytope and Pauli simplex facets.

By comparing the two l_1 distances of $\vec{\lambda}$ to F_j and $\Sigma_{r,s}$ one yields a natural measure for the degree by which quasipinning of D_j exceeds the quasipinning of the Pauli exclusion principle. This gives rise to the important definition of the Q_j -measures:

$$Q_j(\vec{\lambda}) := -\log_{10} \left(\frac{D_j(\vec{\lambda})}{c_j dist_1(\vec{\lambda}, \Sigma_{r,s})} \right). \quad (2.60)$$

Analogously to the measure of a global minimal distance D_{min} (2.44), one can define the global Q -measure:

$$Q := \max_j (Q_j). \quad (2.61)$$

Let us consider three examples (cf. Appendix A). For the GPC $D_{58}^{(3,10)}$ we find

$$Q_{58}(\vec{\lambda}) = -\log_{10} \left(\frac{12 D_{58}(\vec{\lambda})}{29 dist_1(\vec{\lambda}, \Sigma_{1,3})} \right). \quad (2.62)$$

For $D_{40}^{(3,10)}$ two minimal pairs (r, s) exist and thus we use the maximum of the distances between $\vec{\lambda}$ and $\partial\Sigma$:

$$Q_{40}(\vec{\lambda}) = -\log_{10} \left(\frac{D_{40}(\vec{\lambda})}{\max(dist_1(\vec{\lambda}, \Sigma_{0,4}), \frac{1}{2}dist_1(\vec{\lambda}, \Sigma_{1,1}))} \right). \quad (2.63)$$

If a GPC facet does not intersect with any facet $\Sigma_{r,s}$, i.e. if it does not even contain the Hartree-Fock point, then we replace $dist_1(\vec{\lambda}, \Sigma_{r,s})$ by the natural length scale of the Pauli hypercube 1. For instance the GPC $D_{15}^{(3,10)}$ gives rise to:

$$Q_{15}(\vec{\lambda}) = -\log_{10} \left(\frac{5 D_{15}(\vec{\lambda})}{3} \right). \quad (2.64)$$

Let us once again stress the meaning of Q . For any NONs $\vec{\lambda}$, a value $Q(\vec{\lambda})$ means that the encountered quasipinning of GPCs is stronger by a factor of $10^{Q(\vec{\lambda})}$ than one could expect from the quasipinning of the Pauli exclusion principle. Anticipating the results of the next chapter, we shall say that if $Q \lesssim 1$ quasipinning becomes *trivial* and if $Q \gtrsim 2$ it becomes *non-trivial*.

Furthermore, Q also has an operational meaning. Recall the selection rule on the expansion coefficients of (quasi-)pinned states, Cor. 1. A similar relation holds for the coefficients of the states that are (quasi-)pinned by the Pauli exclusion principle constraint $S_{r,s}$, giving rise to the bounds:

$$\alpha_{low} S_{r,s}(\vec{\lambda}) \leq 1 - |\langle \psi_N | P_{\mathcal{I}_{S_{r,s}}} | \psi_N \rangle|^2 \leq \alpha_{top} S_{r,s}(\vec{\lambda}), \quad (2.65)$$

where the prefactors α_{low} and α_{top} are strictly positive and $P_{\mathcal{I}_{S_{r,s}}}$ denotes the projector of the respective N -fermion state $|\psi_N\rangle$ onto the subspace of Slater determinants selected by pinning of $S_{r,s}$. These are all Slater determinants which contain all r natural orbitals associated with the NONs $\lambda_1 \dots \lambda_r$, but none of the natural orbitals related to the NONs $\lambda_{d-s+1} \dots \lambda_d$. By taking the ratio of relation (2.65) with its analogue for a GPC D_j , one finds:

$$\beta_{low} \times 10^{-Q_j(\vec{\lambda})} \leq \frac{1 - |\langle \psi_N | P_{D_j} | \psi_N \rangle|^2}{1 - |\langle \psi_N | P_{\mathcal{I}_{S_{r,s}}} | \psi_N \rangle|^2} \leq \beta_{top} \times 10^{-Q_j(\vec{\lambda})}. \quad (2.66)$$

The Q -parameter thus provides insight into how far quasipinning of a GPC implies additional structural simplifications on the N -fermion wave function.

In the next chapter, we are going to present model systems for which we demonstrate the evaluation of the Q -measure. This will allow us to access whether the encountered absolute quasipinning D_{min} is trivial or non-trivial.

Chapter 3

Quasipinning in physical model systems

In the previous chapter, we have discussed the remarkable discovery of GPCs. Generally, these constraints can be expected to be of particular physical relevance due to a number of reasons. For example, in formalisms such as reduced density matrix functional theory (RDMFT) the variation of the effective energy functional is usually carried out over the domain of 1-RDOs which is solely constrained by the Pauli exclusion principle (2.26).¹ Only recently, Theophilou et al. [96] have found that restricting the variation domain by the GPCs leads to significantly different estimations of the energy values. GPCs might further play a role in modified master equations for the dynamics of fermionic NONs. Another possible instance for the relevance of the GPCs is given by the (quasi-)pinning effect, which has been introduced and discussed in the previous chapter. Recall that the NONs of (quasi-)pinned systems exhibit constraints on their dynamical evolution and that the respective N -particle states have a significantly simplified structure. Hence, the study of the (quasi-)pinning effect and its occurrence in physical systems has become a subject of growing interest among many branches of physics and quantum chemistry [52, 7, 18, 84, 86, 9, 96, 64, 85]. Despite deserving credit for taking the first steps in a new field, those works have not yet investigated models with infinite dimensional one-particle Hilbert spaces and higher spatial dimensions resembling situations found in numerous realistic physical systems. Furthermore, little if anything has been understood about the origin of (quasi-)pinning.

In this chapter, we are going to present results of systematic studies on the occurrence and behaviour of (quasi-)pinning in representative physical model systems. In Ref. [87], evidence for remarkably strong δ^8 -quasipinning was found in the model

¹For a review on RDMFT and density functional theory (DFT) see, e.g., Refs. [22, 70, 77].

system of so-called Harmonium of three spin-polarised fermions in one spatial dimension. We shall extend this result and systematically explore the quasipinning in systems of higher particle numbers, higher numbers of spatial dimensions, dimensional crossovers and finite degrees of spin polarisation. The results indicate that quasipinning becomes weaker when the dimensionality of the system is increased, but grows stronger with the number of particles and the degree of polarisation. Moreover, in their entirety the results give rise to the notion of specific ‘active spaces’ of NONs and the existence of a ‘microscopic Pauli pressure’. Supposedly, this ‘pressure’ is at the origin of quasipinning and forces the $\vec{\lambda}$ -vector towards the boundary of the polytope. Throughout all investigations, the concepts for conclusive pinning analyses presented in the previous chapter will be applied.

For all physical cases mentioned above, we shall in addition study the relevance of the computed quasipinning beyond the respective quasipinning of the Pauli exclusion principle. In order to do so, we shall make use of the Q-measure introduced in the previous section.

We start by introducing and motivating the model system of Harmonium in Sec. 3.1 and derive its N -particle ground state. Thereafter, we shall determine the respective 1-RDO and its NONs, and discuss the required methods for the truncation of the $\vec{\lambda}$ -vector. In Sec. 3.3, quasipinning in one-dimensional N -Harmonium will be studied. Special attention will be directed towards the validity of the pinning analyses and the applied methods of truncation. Following that, quasi-one-dimensional Harmonium will be considered in Sec. 3.4. In the next section, higher dimensions and dimensional crossovers will be closely examined. In the last section, we are going to investigate quasipinning in systems of spinful fermions.

The results of my research presented in this chapter have been published in Refs. [93, 95].

3.1 The model system and its ground state

In this section we introduce the model system of Harmonium in arbitrary spatial dimensions. The structure of its ground state will be thoroughly examined and a concise definition of all coupling parameters will be provided.

Consider a system of N identical (yet spinless) particles of mass m , which are confined in an n -dimensional (not necessarily isotropic) harmonic trapping potential. The potential may be characterised by its n trapping frequencies $\{\omega^{(\alpha)}\}_{\alpha=1}^n$. Further

assume that the particles exhibit a harmonic particle-particle interaction of strength K . Consequently, the Hamiltonian reads:

$$H_N = \sum_{i=1}^N \left(\frac{\vec{p}_i^2}{2m} + \frac{m}{2} \vec{x}_i^t \Omega \vec{x}_i \right) + \frac{K}{2} \sum_{1 \leq i < j \leq N} (\vec{x}_i - \vec{x}_j)^2. \quad (3.1)$$

The quantities $\vec{p}_i = (p_i^{(\alpha)})_{\alpha=1}^n$ and $\vec{x}_i = (x_i^{(\alpha)})_{\alpha=1}^n$ represent the momentum and position operators of the i -th particle, respectively, and $\Omega \equiv \text{diag}(\omega_1^2, \dots, \omega_n^2)$. In this thesis, the N -fermion system associated with this Hamiltonian is referred to as Harmonium.²

In Ref. [56], the Harmonium Hamiltonian was shown to emerge as an effective model when a harmonic approximation is applied to systems of harmonically confined interacting particles. A good example for the success of this approximation is given by the effective description of quantum dots where the Coulomb interaction between the electrons is screened (see Ref. [44]). Moreover, the Harmonium model allows one to study the emergence of shell structures in atoms (see, e.g., Ref. [78]) and nuclei (see, e.g., Ref. [109]). Last but not least, the model was also found to apply to trapped ultracold gases in which the two-body interactions are tuneable [105, 11, 20]. In particular, this encompasses transitions from repulsive to attractive interactions.

In the context of our research, the Harmonium model offers a number of important advantages, too. In order to analytically investigate the occurrence of quasipinning, a system must permit the *analytical* execution of all of the following steps:

1. computation of the many-body eigenstates in a system of *interacting fermions* (see, e.g. Refs. [102, 87, 83, 4]),
2. tracing out $N - 1$ particles (i.e. calculating analytically $(N - 1)n$ integrals),
3. diagonalising the 1-RDO, either analytically in the regime of weak couplings or exact numerically for medium and strong couplings.

While all three steps can be carried out for Harmonium, none of them is tractable for most continuous physical models.

A priori, the Hamiltonian (3.1) acts as an operator on the N -particle Hilbert space $\mathcal{H}_N = \bigotimes_{i=1}^N \mathcal{H}_1$ (2.2), where the one-particle Hilbert space $\mathcal{H}_1$ is given by

²The term of Harmonium has seen ambiguous usage in the literature. Whereas some authors consider it to be a system of N harmonically interacting particles in a harmonic external trapping potential (see, e.g., Refs. [48, 8]), others use it to refer to a system of N particles in a harmonic trap which interact via Coulomb forces (see, e.g., Ref. [23]).

$\mathcal{H}_1 = L_2(\mathbb{R}^n)$. When taking into account the spin degree of freedom in Sec. 3.6, the one-particle Hilbert space will be modified to $\mathcal{H} = L_2(\mathbb{R}^n) \otimes \mathbb{C}^2$.

Observe that H_N remains invariant under arbitrary permutations of the particles. In particular, this allows us to treat the N particles as indistinguishable fermions and thus restrict the Hamiltonian (3.1) to the subspace of antisymmetric states $\mathcal{A}_N \mathcal{H}_N \equiv \mathcal{H}_N^{(f)}$, as defined in Eq. (2.5). In order to derive the set of fermionic eigenstates of the Hamiltonian (3.1) we therefore may initially derive the set of all N -particle eigenstates followed by a projection onto $\mathcal{A}_N \mathcal{H}_N$.

We shall now present a theorem on the general form and structure of the fermionic ground state in Harmonium. A proof of this theorem may be found in the appendix, Sec. B.1. As a first step, it is instructive to look at the Harmonium ground state under zero particle-particle interaction, $K = 0$. In that case the time-independent Schrödinger equation associated with the Hamiltonian (3.1) reduces to N uncoupled one-particle eigenvalue problems of the form

$$\left(\frac{\vec{p}^2}{2m} + \frac{1}{2} m \vec{x}^t \Omega \vec{x} \right) \chi = \varepsilon \chi. \quad (3.2)$$

This specific equation is solved by the n -dimensional Hermite functions

$$\phi_{\boldsymbol{\mu}}^{(\boldsymbol{l})}(\vec{x}) \equiv \prod_{\alpha=1}^n \varphi_{\mu^{(\alpha)}}^{(l^{(\alpha)})}(x^{(\alpha)}) \quad (3.3)$$

with corresponding energy eigenvalues

$$\varepsilon_{\boldsymbol{\mu}} = \sum_{\alpha=1}^n \left(\mu^{(\alpha)} + \frac{1}{2} \right) \hbar \omega^{(\alpha)}. \quad (3.4)$$

Here, $\varphi_m^{(l^{(\alpha)})}$ denotes the m -th Hermite function in one dimension with natural length scale $l^{(\alpha)} \equiv \sqrt{\frac{\hbar}{m\omega^{(\alpha)}}}$, $\boldsymbol{\mu} \equiv (\mu^{(\alpha)})_{\alpha=1}^n$ and $\boldsymbol{l} \equiv (l^{(\alpha)})_{\alpha=1}^n$.

It follows that the many-fermion eigenstates of the Hamiltonian (3.1) with $K = 0$ can be written as Slater determinants of the single-particle states (3.3). These ‘configuration states’ are characterised by a respective distribution of N particles on N different states $\phi_{\boldsymbol{\mu}}^{(\boldsymbol{l})}$. In particular, this applies to the ground state which is obtained by choosing the N different one-particle states with lowest one-particle energies $\varepsilon_{\boldsymbol{\mu}}$, and constructing their Slater determinant according to Pauli’s exclusion principle.

In general physical systems, the elegance of the one-particle description of many-body energy eigenstates can not be retained when particle-particle interactions are incorporated into the model. It thus comes as a surprise that at least the ground

state of Harmonium for $K \neq 0$ still permits the usage of the convenient one-fermion picture:³

Theorem 3

The N -fermion ground state $\Psi^{(f)}$ of the Harmonium model (3.1) is given by

$$\Psi^{(f)}(\vec{x}_1, \dots, \vec{x}_N) = \mathcal{N} \begin{vmatrix} \phi_{\mu_1}^{(\tilde{l})}(\vec{x}_1) & \dots & \phi_{\mu_1}^{(\tilde{l})}(\vec{x}_N) \\ \vdots & & \vdots \\ \phi_{\mu_N}^{(\tilde{l})}(\vec{x}_1) & \dots & \phi_{\mu_N}^{(\tilde{l})}(\vec{x}_N) \end{vmatrix} \times e^{\vec{X}^t \mathbf{B} \vec{X}}, \quad (3.5)$$

with $\vec{X} \equiv \frac{1}{N}(\vec{x}_1 + \dots \vec{x}_N)$ the centre-of-mass vector, $\mathbf{B} \equiv \text{diag}(B^{(1)}, \dots, B^{(n)})$, $B^{(\alpha)} \equiv \frac{N}{2} \left(\frac{1}{(\tilde{l}^{(\alpha)})^2} - \frac{1}{(l^{(\alpha)})^2} \right)$, $\tilde{\omega}^{(\alpha)} \equiv \sqrt{(\omega^{(\alpha)})^2 + \frac{NK}{m}}$, $\tilde{l}^{(\alpha)} \equiv \sqrt{\frac{\hbar}{m\tilde{\omega}^{(\alpha)}}}$ and $\mathcal{N}$ representing a normalisation constant. The corresponding energy eigenvalue reads

$$E_{\mu_1, \dots, \mu_N} \equiv \sum_{i=1}^N \tilde{\varepsilon}_{\mu_i}, \quad (3.6)$$

where the functionals $\tilde{\varepsilon}_{\mu_i}$ are defined similar to those in Eq. (3.4):

$$\tilde{\varepsilon}_{\mu_i} := \sum_{\alpha=1}^n \left(\mu^{(\alpha)} + \frac{1}{2} \right) \hbar \omega^{(\alpha)}. \quad (3.7)$$

The quantum number vectors $\mu_1, \dots, \mu_N$ in Eq. (3.5) are determined by the requirement to simultaneously comply with the following two conditions:

1. the energy functional E (3.6) attains its minimal allowed value at $\mu_1, \dots, \mu_N$,
2. all μ_i are different, i.e. they respect a form of an exclusion principle.⁴

Because the proof of Thm. 3 is not trivial, it shall be elaborated in the appendix, Sec. B.1. Notice that the simple structure of the Harmonium ground states as presented in Thm. 3 does generally not extend to the excited states. It is thus not possible to derive the form of the excited states by filling ‘boxes’ of higher energy and multiplying the associated Slater determinant with the Gaussian factor in Eq. (3.5). Instead we have to incorporate several different Slater determinants, which account for the increasing correlations within the system.

³We remark that multi-dimensional Harmonium in isotropic traps, $\omega^{(1)} = \dots = \omega^{(n)}$, has already been considered in Ref. [102]. However, no constructive proof has been provided.

⁴Note that this exclusion principle should not be confused with Pauli’s exclusion principle which applies to the entire wave function. Here, the constraint of two μ_i being different only applies to the first factor of the wave function (3.5). In the same respect, the notion of distributing N fermions on N places is more of an illustrative character.

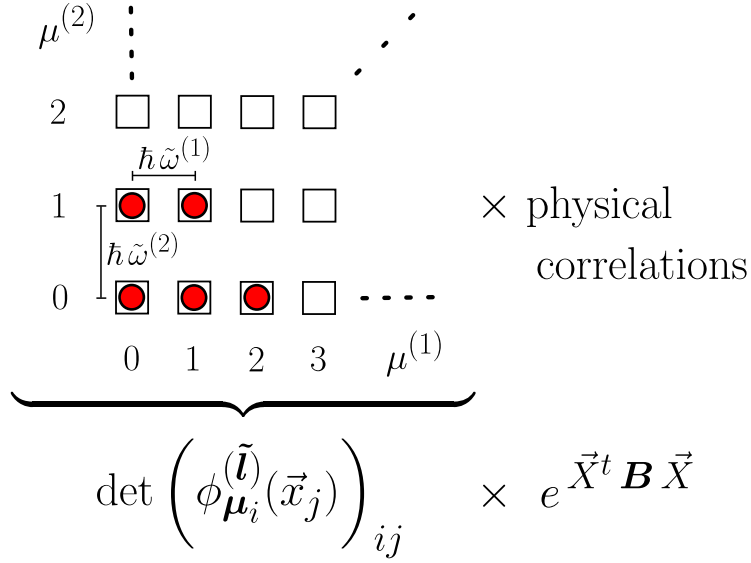


Figure 3.1: Graphical illustration of the fermionic ground state wave function $\Psi^{(f)}$ for the exemplary case of $N = 5$ fermions in $n = 2$ spatial dimensions. The scheme depicts the notion of $\Psi^{(f)}$ being given by a single Slater determinant times the factor of $e^{\vec{X}^t \mathbf{B} \vec{X}}$, which accounts for the physical correlations. Here, $\vec{X} \equiv \frac{1}{N}(\vec{x}_1 + \dots \vec{x}_N)$ represents the centre-of-mass coordinate. The Slater determinant can be derived by filling N ‘boxes’ with N particles. Each box is labelled by a quantum number $\vec{\mu} = (\mu_1, \dots, \mu_n)$ and describes a one-particle state in an n -dimensional harmonic oscillator with frequencies $\tilde{\omega}^{(\alpha)}$, $\alpha = 1, \dots, n$.

Let us now consider a graphical illustration of these ideas in Fig. 3.1. On the left, a scheme of boxes which correspond to the energy functionals in Eq. (3.7) is shown. The two conditions set out in Thm. 3 are met by successively filling these boxes with N particles starting from the left lower corner and avoiding double occupancies. The ground state wave function is then derived by taking the Slater determinant of the respective functions $\phi_{\boldsymbol{\mu}}^{(\tilde{l})}$ and multiplying it with a factor of $e^{\vec{X}^t \mathbf{B} \vec{X}}$. Note that it is this factor which solely accounts for the non-trivial physical correlations, whereas the Slater determinant only induces exchange-related correlations. Fig. 3.1 explicitly depicts the example of $N = 5$ fermions in two-dimensional Harmonium for which the occupied ‘boxes’ are given in terms of the ‘configuration’ $\mathcal{C} = \{\{0, 0\}, \{1, 0\}, \{0, 1\}, \{2, 0\}, \{1, 1\}\}$.

We see that the Harmonium ground state for finite interaction bears resemblance with the ground for vanishing interaction. More precisely, both states only differ by the correlation term $e^{\vec{X}^t \mathbf{B} \vec{X}}$ and the modified natural length scales $\tilde{l}^{(\alpha)}$ of the Hermite functions $\phi_{\boldsymbol{\mu}}^{(\tilde{l})}$. The latter gives rise to a specific distinctiveness of ground

states in the finite interaction regime. If some of the external parameters K and $\omega^{(\alpha)}$ are tuned, the structure of the ground state can abruptly change at certain critical values. Consider the energy ratios $\tilde{\epsilon}_{\boldsymbol{\mu}}/\tilde{\epsilon}_{\boldsymbol{\mu}'}$ which correspond to the ratios of distances between the ‘boxes’ in different directions $\alpha = 1 \dots n$ (cf. Fig. 3.1). The tuning of the external parameters changes these energy ratios, and it thus becomes possible that the N -th and $(N+1)$ th lowest energy levels $\tilde{\epsilon}_{\boldsymbol{\mu}}$ cross. In turn, the initial configuration $\{\boldsymbol{\mu}_1, \dots, \boldsymbol{\mu}_N\}$ must be changed in order for the $\boldsymbol{\mu}_i$ to comply with the requirement for energy minimisation set out in Thm. 3.

An important example of such crossings occurs when one of the harmonic trapping frequencies $\omega^{(\alpha)}$ is increasingly detuned such that the confining potential becomes highly anisotropic. As a consequence, the motion in the α -direction is eventually frozen. If, for instance, one increases $\omega^{(2)}$ in the example set out in Fig. 3.1, then the ground state configuration changes to $\{\{0, 0\}, \{1, 0\}, \{2, 0\}, \{0, 1\}, \{3, 0\}\}$ and finally becomes $\{\{0, 0\}, \{1, 0\}, \{2, 0\}, \{3, 0\}, \{4, 0\}\}$, which corresponds to quasi-one-dimensionality of the system (cf. Sec. 3.4).

At this point, it is instructive to compare the fermionic ground state $\Psi^{(f)}$ to the bosonic ground state $\Psi^{(b)}$ of the Hamiltonian (3.1). Similar to the fermionic case, the bosonic ground state can also be understood with the aid of the ‘box picture’. One has to distribute N bosons on the lowest energy level, given by $\boldsymbol{\mu} \equiv (0, \dots, 0) \equiv \mathbf{0}$, and multiply the resulting product state with $e^{\vec{X}^t \mathbf{B} \vec{X}}$. This leads to the following form of $\Psi^{(b)}$:

$$\Psi^{(b)}(\vec{x}_1, \dots, \vec{x}_N) \sim \left(\prod_{i=1}^N \phi_{\mathbf{0}}^{(\tilde{l})}(\vec{x}_i) \right) \times e^{\vec{X}^t \mathbf{B} \vec{X}} \sim \left(\prod_{i=1}^N e^{-\vec{x}_i \mathbf{A} \vec{x}_i} \right) \times e^{\vec{X}^t \mathbf{B} \vec{X}}. \quad (3.8)$$

Here, $\mathbf{A} \equiv \text{diag}(A^{(1)}, \dots, A^{(n)})$ and $A^{(\alpha)} \equiv \frac{1}{2(\tilde{l}^{(\alpha)})^2}$. For details, see appendix, Sec. B.1.

Before addressing the reduced one-particle information of Harmonium ground states in the following section, it is worth taking a closer look at their symmetries. First, note that for arbitrary sets of parameters, K and $\{\omega^{(\alpha)}\}_{\alpha=1}^n$, the Hamiltonian (3.1) remains invariant when the α -coordinates of all N particles are simultaneously reflected, $P^{(\alpha)} : x_i^{(\alpha)} \rightarrow -x_i^{(\alpha)}$, $i = 1, \dots, N$. Specifically:

$$[\hat{H}, U(P^{(\alpha)})^{\otimes N}] = 0. \quad (3.9)$$

In this equation, U represents the unitary operator on the one-particle Hilbert space, which mediates the spatial reflection. Naturally, the symmetry of the Hamiltonian enters the respective ground state: $U(P^{(\alpha)})^{\otimes N} \Psi^{(f)} = \pm \Psi^{(f)}$.

Second, if the system is isotropic in particular spatial dimensions, e.g. if two trapping frequencies coincide, $\omega^{(\alpha)} = \omega^{(\alpha')}$, then the Hamiltonian exhibits another symmetry in form of an invariance under spatial rotations in the $\alpha - \alpha'$ -plane: $R^{(\alpha, \alpha')} : (x_i^{(\alpha)}, x_i^{(\alpha')})^t \rightarrow R(x_i^{(\alpha)}, x_i^{(\alpha')})^t$, $R \in SO(2)$. Clearly, the scheme also applies to arbitrary numbers of spatial isotropies. Note further that it is this spatial degeneracy which gives rise to the interesting property of emerging energy shell structures in isotropic Harmonium (see also Ref. [78]).

3.2 One-particle reduced density operator and natural occupation numbers

In this section, we derive the 1-RDO of the N -Harmonium ground state which will lay out the basis for all subsequent pinning analyses. We shall first address general structural properties of the 1-RDO which arise from underlying symmetries of the model Hamiltonian. This will be followed by a brief review on the form of the 1-RDO in one-dimensional Harmonium, which has already been obtained in Refs. [87, 83]. Finally, the general form of the ground state 1-RDO for N -Harmonium in arbitrary spatial dimensions will be presented and discussed.

3.2.1 General considerations

The fermionic 1-RDO, $\rho_1^{(f)}$, of a pure quantum state has been defined in Eq. (2.12). Throughout the rest of this chapter it shall be normalised to N and its lower index shall be omitted where no confusion with ρ_N can arise.

At the end of the previous section, we have explored symmetries of the Harmonium model. It is well-known that one-particle symmetries of the N -fermion state are inherited by the respective 1-RDO (cf. Ref. [29]). Specifically, consider a one-particle symmetry of the N -particle state $|\Psi^{(f)}\rangle$ which is associated with the unitary operator $G = g^{\otimes N}$. Here, g denotes a unitary operator on the one-particle Hilbert space $\mathcal{H}_1$. For G to be a symmetry we have

$$G |\Psi^{(f)}\rangle = e^{i\zeta} |\Psi^{(f)}\rangle, \quad (3.10)$$

with $\zeta \in \mathbb{R}$. By the definition and nature of the partial trace this relation implies that g and $\rho^{(f)}$ commute:

$$[g, \rho^{(f)}] = 0. \quad (3.11)$$

The operators g and $\rho^{(f)}$ therefore share a common system of eigenstates, which in turn implies that the 1-RDO, when regarded as a matrix in the basis of g -symmetry-adapted states⁵, becomes block diagonal.

For example, consider a translationally invariant system of N spinful fermions. The natural orbitals will be given by direct products of the Bloch states with spin states. Hence, the natural orbitals and occupation numbers gain physical significance by describing the one-particle momentum distribution.

In the case of N -Harmonium, the ground state symmetry under spatial reflection, Eq. (3.9), permits a sophisticated choice of parity-adapted basis elements, which will block-diagonalise the 1-RDO and make its diagonalisation easier.

3.2.2 One-particle reduced density operator of the Harmonium ground state

We shall now discuss the 1-RDO of the one-dimensional N -Harmonium ground state and present the tools that are required to compute its truncated spectrum. Then the extension of these concepts to N -Harmonium in arbitrary spatial dimensions shall be considered. In the following, it will be convenient to introduce the dimensionless interaction strengths

$$\kappa^{(\alpha)} := \frac{NK}{m(\omega^{(\alpha)})^2} = \left(\frac{l^{(\alpha)}}{\tilde{l}^{(\alpha)}} \right)^4 - 1. \quad (3.12)$$

For one-dimensional Harmonium the index of κ becomes redundant and shall be omitted. Observe further that the spectrum and the eigenstates of the Harmonium Hamiltonian (3.1) only depend on the ratios of K to $(\omega^{(\alpha)})^2$ and will thus merely be functions of the $\kappa^{(\alpha)}$.

The fermionic 1-RDO $\rho(x, y)$ in spatial representation was derived in Ref. [83] by integration of $|\Psi^{(f)}|^2$ over $N - 1$ particle positions. It becomes the product of a symmetric polynomial F and a Gaussian:

$$\rho^{(f)}(x, y) = F(x, y) e^{-\alpha(x^2+y^2)+\beta xy}. \quad (3.13)$$

The coefficients of F , and the parameters α and β depend on the particle number N , the trapping frequency ω and the interaction strength K .⁶

⁵i.e. eigenstates of g

⁶The explicit form of these quantities may be found in the appendix, Sec. B.2, where the general form of the fermionic 1-RDO is derived.

In Sec. 3.1, Eq. (3.8), the form of the bosonic N -Harmonium ground state was recognised to differ from the fermionic ground state only by a polynomial prefactor. Integration over $N - 1$ particle positions yields the bosonic 1-RDO in spatial representation (cf. appendix, Sec. B.2)

$$\rho^{(b)}(x, y) = \sqrt{\frac{2\alpha - \beta}{\pi}} e^{-\alpha(x^2 + y^2) + \beta xy}, \quad (3.14)$$

which resembles the fermionic 1-RDO up to the polynomial prefactor F .

The bosonic 1-RDO is further recognised as the spatial representation of the Gibbs state (see, e.g., Refs. [36, 84]) and can thus be analytically diagonalised:

$$\rho^{(b)}(x, y) = c(\kappa) \sum_{k=0}^{\infty} \frac{q(\kappa)^k}{k!} \varphi_k^{(L)}(x) \varphi_k^{(L)}(y). \quad (3.15)$$

The eigenstates are given by the Hermite functions $\{\varphi_k^{(L)}(x)\}_{k=0}^{\infty}$ with natural length scale $L \equiv \sqrt{l\tilde{l}} \left[\frac{(N-1)\tilde{l}^2 + l^2}{\tilde{l}^2 + (N-1)l^2} \right]^{\frac{1}{4}}$. The prefactor reads $c(\kappa) \equiv N(1 - q(\kappa))$ and the decay factor $q(\kappa)$ becomes:

$$q(\kappa) = 1 - \frac{2N}{N + \sqrt{N^2 - (N-1)[2 - (1+\kappa)^2 - 1/(1+\kappa)^2]}}. \quad (3.16)$$

Unlike for bosons, it is more difficult to determine the spectrum of the fermionic 1-RDO (3.13) as this operator cannot analytically be diagonalised. Therefore, one either has to resort to numerical techniques or to a perturbative expansion of $\rho^{(f)}$ in the regime of small coupling strengths. Both methods initially require one to derive a suitable matrix representation of the density kernel $\rho^{(f)}$. Due to the structural similarities between the bosonic and fermionic 1-RDOs, it proves advantageous to use the basis of bosonic natural orbitals, i.e. the Hermite functions:

$$(\rho^{(f)})_{kn} \equiv (\langle \varphi_k^{(L)} | \rho^{(f)} | \varphi_n^{(L)} \rangle)_{k,n \geq 0}. \quad (3.17)$$

Note that the resulting (infinite-dimensional) matrix encompasses a number of properties:

First, since the Hermite functions have definite parity, $\varphi_k^{(L)}(-x) = (-1)^k \varphi_k^{(L)}(x)$, the matrix $(\rho^{(f)})_{kn}$ can be decomposed into two diagonal blocks by sorting the basis elements with respect to even and odd degree k (cf. Sec. 3.2.1):

$$\rho^{(f)} = \rho_{\text{even}}^{(f)} \oplus \rho_{\text{odd}}^{(f)}. \quad (3.18)$$

Hence, when the basis elements are ordered as in Eq. (3.17), the matrix elements vanish, $(\rho^{(f)})_{kn} = 0$, whenever $k + n$ is odd.

Second, $(\rho^{(f)})_{kn}$ has a band structure: By expressing x, y in terms of ladder operators of a harmonic oscillator with length scale L , and noting that the polynomial prefactor F has a finite degree $2(N-1)$, one finds:

$$(\rho^{(f)})_{kn} = 0, \quad \text{whenever } |k - n| > 2(N-1). \quad (3.19)$$

Third, as a consequence of the Gaussian in the expression of $\rho^{(f)}(x, y)$ (3.13), the matrix elements of $(\rho^{(f)})_{kn}$ decay with powers of the decay factor $q(\kappa)$:

$$(\rho^{(f)})_{kn} \leq \text{const} \times q(\kappa)^{\max(k, n)}. \quad (3.20)$$

This relation paves the way for the derivation of the truncated $\vec{\lambda}$ -vector as shall now be worked out in more detail.

The numerical computation of the R largest NONs of a fermionic 1-RDO with fixed interaction strength κ can be accomplished by truncating the upper-left $R \times R$ block of the matrix $\rho_{kn}^{(f)}$ and determining its eigenvalues $\vec{\lambda}^{(R)} \equiv (\lambda_i^{(R)})_{i=1}^R$. The decaying behaviour of the matrix (3.20), together with a norm estimate described in Ref. [79], impose an upper bound on the deviation of $\vec{\lambda}^{(R)}$ from the exact $\vec{\lambda}$ -vector:

$$\|\vec{\lambda} - \vec{\lambda}^{(R)}\|_1 \leq \text{const} \times q(\kappa)^{R+1}, \quad (3.21)$$

Here it is understood that $\vec{\lambda}^{(R)}$ is the natural extension of $\vec{\lambda}^{(R)}$ to an infinite dimensional vector with $\lambda_i^{(R)} = 0$ for $i > R$. For any arbitrary but fixed interaction strength κ , the decay factor q determines the required size of truncation for a desired level of accuracy in the natural occupation numbers. The dependence of q on κ is shown in Fig. 3.2.

For small couplings one can further use perturbative methods to derive an expression for $\vec{\lambda}$ -vectors close to the Hartree-Fock point associated with $K = 0$ (see Eq. (2.43)). Consider the expansion of $q(\kappa)$ (cf. Eq. (3.16)) in the regime of weak couplings:

$$q(\kappa) = \frac{N-1}{N^2} \kappa^2 + \frac{N-1}{N^2} \kappa^3 + \mathcal{O}(\kappa^4), \quad (3.22)$$

In conjunction with the decay relation (3.20), this permits an expansion of the reduced one-particle matrix $(\rho^{(f)})_{kn}$ in a power series of κ :

$$\rho^{(f)} \equiv \sum_{n=0}^{\infty} \frac{1}{n!} \rho_{(n)} \kappa^n. \quad (3.23)$$

Note that as a consequence of the decay relation, all expansion coefficient matrices $\rho_{(n)}$ have finite rank. By using degenerate Rayleigh-Schrödinger perturbation theory

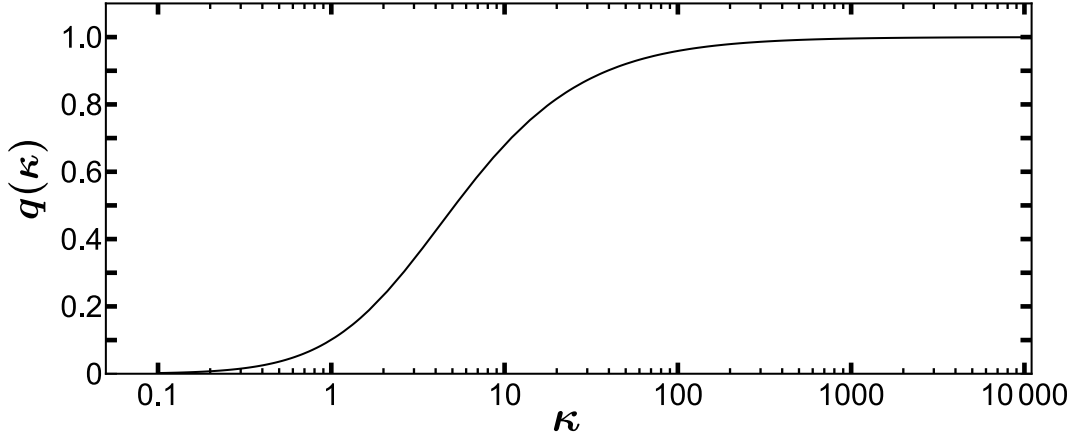


Figure 3.2: Dependence of the decay constant $q(\kappa)$, defined in Eq. (3.16), on the interaction strength κ .

one can therefore determine an analytical expression of the $\vec{\lambda}$ -vector to arbitrary order in the perturbative interaction strength parameter.

Having thoroughly examined the case of one-dimensional Harmonium it is now possible to generalise the above concepts to Harmonium in arbitrary spatial dimensions. By using the Hubbard-Stratonovitch relation, a straightforward but laborious calculation (see appendix, Sec. B.2) shows that the fermionic 1-RDO of the n -dimensional Harmonium ground state is given by:

$$\rho^{(f)}(\vec{x}, \vec{y}) = F(\vec{x}, \vec{y}) \cdot \rho^{(b)}(\vec{x}, \vec{y}). \quad (3.24)$$

Here, $F(\vec{x}, \vec{y})$ is a multivariate polynomial and $\rho^{(b)}(\vec{x}, \vec{y})$ represents the corresponding bosonic 1-RDO which is given by a product of Gaussians.

Similar to Eq. (3.15), the bosonic 1-RDO becomes diagonal in a product basis of Hermite functions. Again, it proves beneficial to map the density kernel of $\rho^{(f)}(\vec{x}, \vec{y})$ to the reduced density matrix in the product basis of Hermite functions. Following that, one can apply the same concepts as set out after Eq. (3.17) above. Careful attention needs to be paid to the altered decay relation, whose specific form will depend on the ordering of the product basis elements.

In higher dimensional Harmonium, the use of symmetries for an efficient diagonalisation will become more important. Recall that the inversion symmetry could be used to block-diagonalise the 1-RDO in bases with definite parity (cf. Sec. 3.2.1). For instance, as a generalisation of the decomposition (3.18) one finds for two-dimensional Harmonium:

$$\rho^{(f)} = \rho_{ee}^{(f)} \oplus \rho_{eo}^{(f)} \oplus \rho_{oe}^{(f)} \oplus \rho_{oo}^{(f)}, \quad (3.25)$$

where the indices $\mathbf{e}$ and $\mathbf{o}$ denote underlying even and odd parities for the respective dimensions $\alpha = 1, 2$. Decomposition structures, such as (3.25), will help us to significantly simplify the calculation of the eigenvalues of the 1-RDO $\rho^{(f)}$.

Finally, let us consider an alternative definition for a dimensionless interaction parameter δ :

$$\delta^{(\alpha)} := \ln \left(\frac{l^{(\alpha)}}{\tilde{l}^{(\alpha)}} \right) = \frac{1}{4} \ln (1 + \kappa^{(\alpha)}) = \frac{1}{4} \kappa^{(\alpha)} + \mathcal{O}((\kappa^{(\alpha)})^2). \quad (3.26)$$

In Ref. [87], a duality relation for the $\vec{\lambda}$ -vector was observed which we find to extend to Harmonium in arbitrary spatial dimensions. For all $\alpha = 1, 2, \dots, n$, this duality reads

$$\vec{\lambda}(\dots, \delta^{(\alpha)}, \dots) = \vec{\lambda}(\dots, -\delta^{(\alpha)}, \dots). \quad (3.27)$$

If one chooses $\delta^{(\alpha)}$ as the perturbation parameter in the expansion of $\vec{\lambda}$ for small coupling strengths (cf. Eq. (3.23)), then the series will only contain even order terms. This furthermore establishes a one-to-one correspondence between quasipinning in the regimes of attractive interactions ($\tilde{l}^{(\alpha)} > l^{(\alpha)}$) and repulsive interactions ($\tilde{l}^{(\alpha)} < l^{(\alpha)}$).

In the remainder of this chapter we shall explore the realm of quasipinning in various physical situations.

3.3 One-dimensional Harmonium with arbitrary particle numbers

Having developed the tools for computing truncated $\vec{\lambda}$ -vectors in the previous section, we shall now discuss quasipinning in one-dimensional N -Harmonium. In the works of Schilling et al. [87, 84], quasipinning of one-dimensional Harmonium has been investigated by perturbation methods for $N = 3$ particles, and numerically for $N = 4, \dots, 8$ particles. In the present section, the perturbative analysis in the regime of weak couplings shall be extended to higher particles numbers. Thereby, the active space structure conjectured in Ref. [84] (cf. Tab. 3.1) will also be confirmed analytically. In the regime of intermediate and strong couplings, we shall investigate the quasipinning and the validity of the truncation method. Furthermore, the Q-parameter will be used to quantify the relevance of the encountered quasipinning beyond the well-known pinning of the Pauli exclusion principle.

...	λ_{N-3}	λ_{N-2}	λ_{N-1}	λ_N	λ_{N+1}	λ_{N+2}	λ_{N+3}	λ_{N+4}	...
...	κ^8	κ^6	κ^4	κ^4	κ^4	κ^4	κ^6	κ^8	...

Table 3.1: Leading order corrections to the spectrum of the Hartree-Fock point $\vec{\lambda}_{HF}$ (2.43), for the decreasingly-ordered NONs $\lambda_i(\kappa)$ of the N-Harmonium ground state for small coupling κ (also cf. Ref. [84]).

3.3.1 Weak couplings

To begin with, we shall extend the results of Ref. [87] to the 4-Harmonium ground state. For weak couplings we can compute a perturbative series expansion of the $\vec{\lambda}$ -vector in the dimensionless interaction parameter δ (3.26) by applying degenerate Rayleigh-Schrödinger perturbation theory. Up to correction terms of the order $\mathcal{O}(\delta^{10})$, the nine largest NONs read:

$$\begin{aligned}
\lambda_1(\delta) &= 1 - \frac{555}{65536}\delta^8 + \mathcal{O}(\delta^{10}) \\
\lambda_2(\delta) &= 1 - \frac{5}{64}\delta^6 + \frac{11735}{196608}\delta^8 + \mathcal{O}(\delta^{10}) \\
\lambda_3(\delta) &= 1 - \frac{15}{64}\delta^4 + \frac{95}{256}\delta^6 - \frac{30387}{65536}\delta^8 + \mathcal{O}(\delta^{10}) \\
\lambda_4(\delta) &= 1 - \frac{15}{64}\delta^4 + \frac{75}{256}\delta^6 - \frac{63281}{196608}\delta^8 + \mathcal{O}(\delta^{10}) \\
\lambda_5(\delta) &= \frac{15}{64}\delta^4 - \frac{75}{256}\delta^6 + \frac{58361}{196608}\delta^8 + \mathcal{O}(\delta^{10}) \\
\lambda_6(\delta) &= \frac{15}{64}\delta^4 - \frac{95}{256}\delta^6 + \frac{30987}{65536}\delta^8 + \mathcal{O}(\delta^{10}) \\
\lambda_7(\delta) &= \frac{5}{64}\delta^6 - \frac{15455}{196608}\delta^8 + \mathcal{O}(\delta^{10}) \\
\lambda_8(\delta) &= \frac{2835}{65536}\delta^8 + \mathcal{O}(\delta^{10}) \\
\lambda_9(\delta) &= \mathcal{O}(\delta^{10}).
\end{aligned} \tag{3.28}$$

By exploiting the concept of truncation, we shall now perform a pinning analysis for these NONs (also cf. Sec. 2.4):

1. Taking into account terms up to fourth order, $\mathcal{O}(\delta^4)$, the active space is given by $\{\lambda_3, \lambda_4, \lambda_5, \lambda_6\}$, while all other NONs are either 1 or 0. The GPCs for the (2, 4) setting, however, do not comprise inequalities and are therefore trivially satisfied.
2. By considering all terms on the scale of $\mathcal{O}(\delta^6)$, one finds an active space with the size of the Borland-Dennis setting $(N', d') = (3, 6)$ (cf. Eq. (2.31)). The active NONs of this setting, λ'_i , are linked with the $\vec{\lambda}$ -vector (3.28) via $\lambda'_i = \lambda_{i+1}$,

$i = 1, 2, \dots, 6$. Up to order $\mathcal{O}(\delta^8)$, these NONs fulfil the equality constraints of the Borland-Dennis setting (2.31a):

$$\lambda'_1 + \lambda'_6 = \lambda'_2 + \lambda'_5 = \lambda'_3 + \lambda'_4 = 1 + \mathcal{O}(\delta^8). \quad (3.29)$$

The inequality constraint (2.31b) is saturated up to eighth order terms:

$$D^{(3,6)}(\vec{\lambda}') \equiv 2 - (\lambda'_1 + \lambda'_2 + \lambda'_4) = -\frac{47569}{65536}\delta^8 \geq 0. \quad (3.30)$$

Since the truncation error is of the same order, one can conclude that the full spectrum of NONs saturates at least some GPCs of the $(4, \infty)$ setting up to order $\mathcal{O}(\delta^8)$, i.e. $D_{min} \sim \delta^r$, $r \geq 8$. In order to determine whether $r = 8$ is the leading order degree of the minimal distance, one has to consider even a larger setting.

3. By including all terms up to order $\mathcal{O}(\delta^8)$, one has to analyse the setting $(4, 8)$ of the eight largest NONs in Eqs. (3.28). This setting comprises 14 GPCs in form of proper inequalities (cf. appendix, Sec. A). The pinning analysis establishes true quasipinning of $D_{min} \sim \delta^8$, which is larger than the truncation error of tenth order and thus completes the analysis.

Observe that the derived quasipinning of eighth order is remarkably strong in comparison to the order of the distance between the $\vec{\lambda}$ -vector and the Hartree-Fock point:

$$dist_1(\vec{\lambda}(\delta), \vec{\lambda}_{HF}) \equiv \sum_{i=1}^N (1 - \lambda_i) + \sum_{j=N+1}^{\infty} \lambda_j \sim \delta^4. \quad (3.31)$$

Repeating the same procedure for higher particle numbers $N = 5, \dots, 8$ we obtain perturbation series expansions of the NONs similar to (3.28). The pronounced patterns in the leading order perturbations confirm the hierarchy displayed in Tab. 3.1. Note here that the leading orders of the κ and δ expansion series coincide due to Eq. (3.26). Quasipinning analyses reveal that

$$\begin{aligned} D_{min} &= c_N \delta^{2N} + \mathcal{O}(\delta^{2N+2}) \\ &= d_N \kappa^{2N} + \mathcal{O}(\kappa^{2N+1}), \end{aligned} \quad (3.32)$$

for $4 \leq N \leq 8$, where $d_N = \frac{c_N}{4^{2N}}$. This is the analytical extension to higher particle numbers of the original result of $D_{min} \sim \delta^8$ in Refs. [87, 84] for $N = 3$ particles. Although pinning analyses cannot be performed for particle numbers $N \geq 9$ (yet) due to the lack of knowledge about the required larger settings of GPCs, it is plausible to assume that Eq. (3.32) generalises to arbitrary particle numbers.

λ_1	0.999998533821	λ_6	0.000001455434
λ_2	0.999807955780	λ_7	0.000000028353
λ_3	0.999806535259	λ_8	0.000000000265
λ_4	0.000193443778	λ_9	0.000000000002
λ_5	0.000192047307	...	...

Table 3.2: NONs of the one-dimensional 3-Harmonium ground state at $\kappa = 1$ up to magnitude $\lambda_i \geq 10^{-12}$.

The strong increase of the quasipinning D_{min} with the particle number N , together with the observed hierarchy of NONs (cf. Tab. 3.1), suggests the existence of a ‘microscopic Pauli pressure’. By this notion of a pressure, every additional particle in the trap forces the $\vec{\lambda}$ -vector of the system closer to the boundary of the polytope, and respectively to the boundary of the Pauli simplex Σ .

The result (3.32) is a strong indicator of the absolute influence of the fermionic exchange statistics. To measure its relative influence one has to examine whether the pinning of respective GPCs exceeds the pinning of the Pauli exclusion principle. Due to Eq. (3.31), at least four orders of the quasipinning (3.32) will be trivial. By applying the Q-parameter to NONs in the form of perturbation series expansions, such as (3.28), one yields:

$$Q \sim 2 \log_{10} \delta, \quad (3.33)$$

for $3 \leq N \leq 8$. Consequently, the respective quasipinning (3.32) is non-trivial by two orders in the perturbation parameter.

3.3.2 Intermediate and strong couplings

In the previous section, the results on quasipinning in one-dimensional 3-Harmonium have been analytically extended to higher particle numbers. The applied perturbation methods are valid in the regime of small interaction strengths $\delta \ll 1$. In terms of the alternative interaction parameter κ this regime corresponds to weak physical interactions $\kappa \lesssim 1$, since $\kappa(\delta = 1) \approx 53.6$ due to Eq. (3.26). In principle, the convergence radii of perturbation series expansions of NONs, such as (3.28), may even be of order $\mathcal{O}(1)$ although this could not be verified. We shall now explore quasipinning in the regime of intermediate and strong couplings by numerical diagonalisation of truncated 1-RDOs for various interaction strengths. To confirm the validity of the analysis one has to evaluate the truncation error ΔD_{min} as well. Here we use the

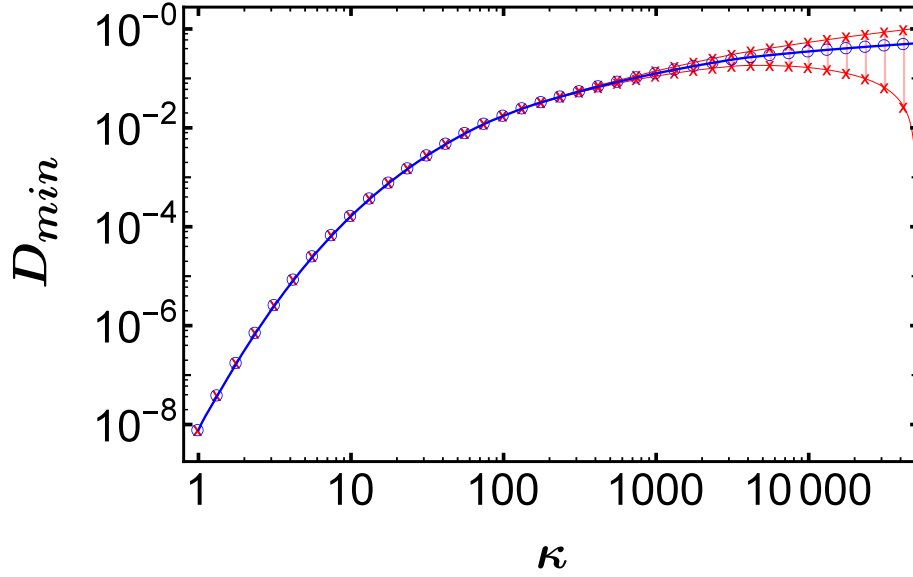


Figure 3.3: Quasipinning exhibited by the 3-Harmonium ground state in one spatial dimension: Numerical data points of minimal l^1 -distance D_{min} of the NONs $\vec{\lambda}$ to polytope boundary $\partial\mathcal{P}$ for intermediate up to very strong interaction strengths (blue circles). Upper and lower error margins (red crosses) within the largest known setting $(N, d) = (3, 11)$ are found negligible for even strong interactions up to $\kappa \approx 5000$.

definition of

$$\Delta D_{min} := \sum_{i=1}^r (1 - \lambda_i) + \sum_{j=d-s+1}^d \lambda_j, \quad (3.34)$$

where r and s are the numbers of neglected NONs close to 1 and 0, respectively. Note that a subtlety in such definition originates from the lack of knowledge about GPCs in the limit of large one-particle Hilbert spaces.

Let us now consider “Lithium-like” 3-Harmonium with $3K = m\omega^2$, i.e. $\kappa = 1$. Numerical diagonalisation of the truncated 1-RDO yields the set of NONs shown in Tab. 3.2. Their values indicate weak correlations. A pinning analysis yields

$$D_{min} = 7.66 \times 10^{-9}, \quad (3.35)$$

which compares with a deviation from the Hartree-Fock point of

$$\text{dist}_1(\vec{\lambda}, \vec{\lambda}_{HF}) = 7.74 \times 10^{-4}. \quad (3.36)$$

By a factor of 10^5 , the $\vec{\lambda}$ -vector lies closer to the boudary of the polytope than to the Hartree-Fock point. The non-triviality of this quasipinning is measured by the Q -parameters as $Q = 1.85$; this means that D_{min} exceeds the pinning of Pauli’s exclusion principle by a factor of $10^{1.85} \approx 71$.

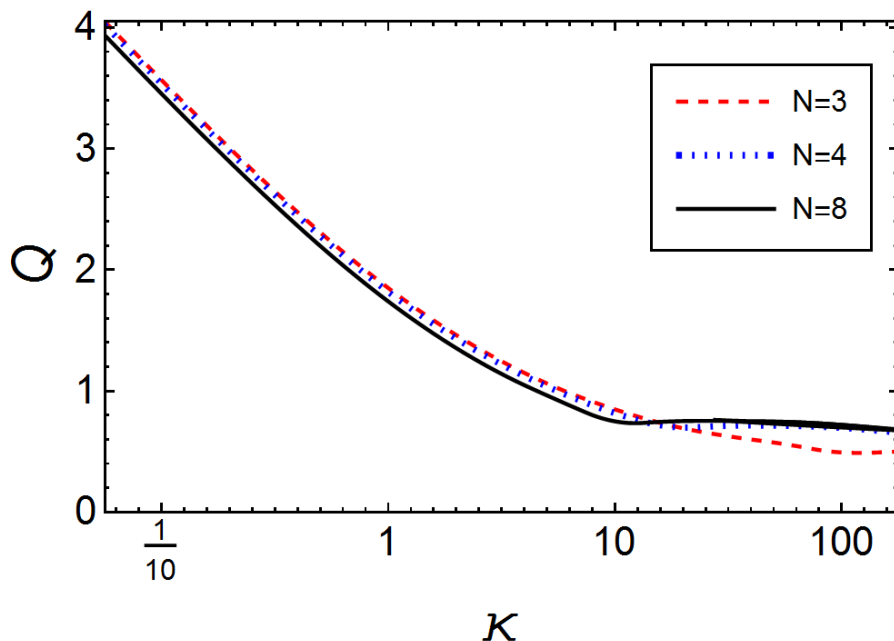


Figure 3.4: Non-triviality of quasipinning: Q -measure for the N -Harmonium ground state with $N = 3, 5, 8$ as function of the coupling κ . Q is seen to be similar for various particle numbers. The logarithmic plot reveals a linear behaviour for small interaction strengths κ . Since the corresponding slope is 2, this confirms that the quasipinning is non-trivial by two orders in κ .

As a next step, one can study quasipinning in the regime of $\kappa \geq 1$ and examine the occurring truncation errors (3.34). The results of an interpolation of minimal distances $D_{min}(\kappa)$ at a set of logarithmically distributed points κ are plotted in Fig. 3.3 (blue circles). The corresponding upper and lower error margins within the largest known setting of GPCs, $(N, d) = (3, 11)$, are marked by red crosses. One finds that the truncation error remains negligible up to strong couplings of $\kappa \lesssim 5000$, which affirms the validity of the respective pinning analyses. For ultra-strong couplings, $\kappa \gtrsim 50000$, the truncation error becomes too large for a conclusive pinning analysis.

Generally, one observes that the quasipinning effect in one-dimensional 3-Harmonium is also present in systems with strong couplings. However, it becomes weaker the more κ is increased and eventually vanishes approaching the scale of the polytope diameter, i.e. $\mathcal{O}(1)$, in the regime of ultrastrong couplings.

For higher particle numbers $4 \leq N \leq 8$, the dependence of D_{min} on κ is similar to the case of $N = 3$.

The non-triviality of the quasipinning is determined by using the Q -parameter. Fig. 3.4 demonstrates that Q diminishes with increasing coupling strengths like $Q \sim$

$-2\log_{10}(\kappa)$ independently of the particle number N in the regime of weak couplings. The minimal distance to the polytope boundary exceeds the saturation of Pauli's exclusion principle constraints by two orders in κ . Furthermore, the results show that the quasipinning remains non-trivial up to intermediate coupling strengths and becomes trivial in the regime of large interaction strengths.

3.4 Quasi-one-dimensional Harmonium

Before investigating truly higher-dimensional systems in later sections, we will now explore the quasipinning behaviour in quasi-one-dimensional systems. This will especially allow us to link outcomes of subsequent analyses to the results of the previous section on strictly one-dimensional Harmonium. By quasi-one-dimensional systems we mean systems in which all but one trapping frequencies have been highly detuned. In addition, we assume those detuned frequencies $\omega^{(2)}, \dots, \omega^{(n)}$ to be identical yielding a hypercylindrical trapping potential. In graphical representations of the Harmonium ground state as shown in Fig. 3.1 this relates to a situation in which the inter-‘box’ spacings $\hbar\tilde{\omega}^{(\alpha)}$ have severely been increased in all but one dimension, $\tilde{\omega}^{(\alpha)}/\tilde{\omega}^{(1)} \gg 1$ for $\alpha = 2 \dots N$. Consequently, only energy levels along the one-axis will be occupied. This resembles the physical situation in which harmonic oscillators in the directions $\alpha \geq 2$ carry no excitations.

Generally, the notion of effective lower dimensionality can be captured more formally as follows. If a configuration has quantum number vectors $\{\boldsymbol{\mu}_i\}_{i=1}^N$ with $\mu_i^{(\alpha)} = 0$ for all $\alpha > n'$ and $i = 1 \dots N$, the fermionic ground state function decomposes into a product of the fermionic ground state function in the first n' dimensions and the bosonic ground state function in the remaining $(n - n')$ dimensions,

$$\Psi_n^{(f)} = \Psi_{n'}^{(f)} \otimes \Psi_{n-n'}^{(b)}. \quad (3.37)$$

Such effective lower dimensionality has structural implications on the fermionic 1-RDO as well: The polynomial F in Eq. (3.24) will not depend on $x_i^{(\beta)}, x_i'^{(\beta)}$ with $i = 1 \dots N$ and $\beta > n'$. Hence, the 1-RDO becomes a product of a fermionic 1-RDO in the first n' dimensions and the bosonic 1-RDO in the remaining $(n - n')$ dimensions,

$$\rho_n^{(f)} = \frac{1}{N} \rho_{n'}^{(f)} \otimes \rho_{n-n'}^{(b)}. \quad (3.38)$$

The factor N originates from the specific normalisation of 1-RDOs, $\text{tr}(\rho) = N$.

As a consequence of Eq. (3.38), the spectrum of $\rho_n^{(f)}$ becomes the product of the spectrum of the lower-dimensional fermionic 1-RDO and the spectrum of the bosonic 1-RDO,

$$\vec{\lambda}_n^{(f)} = \frac{1}{N} \left(\vec{\lambda}_{n'}^{(f)} \times \vec{\lambda}_{n-n'}^{(b)} \right)^\downarrow, \quad (3.39)$$

where ‘ $\downarrow$ ’ denotes decreasing ordering.

These considerations can now be applied to quasi-one-dimensional Harmonium which is achieved for sufficiently large trapping frequency detunings, i.e.

$$\tilde{\omega}^{(\alpha)} > (N-1)\tilde{\omega}^{(1)} \quad \text{for } \alpha \geq 2. \quad (3.40)$$

The corresponding vector of ground state NONs is then given by the product of the spectrum $\vec{\lambda}_1^{(f)}$ of the one-dimensional fermionic 1-RDO and $(n-1)$ spectra $\vec{\lambda}_1^{(b)}$ of the $(n-1)$ decoupled one-dimensional bosonic 1-RDOs. In Sec. 3.2.2 the one-dimensional bosonic 1-RDO was diagonalised in Eq. (3.15). For some coupling strength $\bar{\kappa}$, the spectrum can be read as:

$$\lambda_k^{(b)}(\bar{\kappa}) = N(1 - q(\bar{\kappa})) q(\bar{\kappa})^k, \quad k \in \mathbb{N}_0^+, \quad (3.41)$$

where $q(\bar{\kappa})$ is defined via Eq. (3.16). The coupling strengths $\kappa^{(2)} = \dots = \kappa^{(n)} \equiv \bar{\kappa}$ of the bosonic spectra that correspond to spatial directions $\alpha \geq 2$ can be expressed as a function of $\delta \equiv \delta^{(1)}$ and the trapping frequency ratios $\chi \equiv \omega^{(\alpha)}/\omega^{(1)}$. Further note that with increasing detunings χ the bosonic spectra more and more approach $(N, 0, 0, \dots)$.

Let us apply these general ideas to the exemplary case $N = 3$ and $n = 2$. The spectrum $\vec{\lambda}_1^{(f)}$ was determined in Ref. [87] and is also listed in Appendix B.3. Using the relation for the product spectrum (3.39) and the form of the bosonic spectra (3.41), one can derive the NONs of the quasi-one-dimensional Harmonium ground state. The pinning analysis of the spectra however, is intricate for two reasons.

First, variation of the external parameters δ and χ can and will change the ordering hierarchy of NONs. This in turn changes the quasipinning behaviour as well. Note that similar crossings of NONs have been described for the Hubbard model in Ref. [85]. Second, even when restricting the analysis to regimes with no crossings of NONs, it is difficult to provide an analytical expression for the minimal distance since the specific most saturated GPC associated with D_{min} can change under the tuning of δ and χ .

Hence, it is necessary to divide the parameter space into different regimes, in which the most relevant NONs do not cross. In the following, we will focus on the

regime which comprises the limit $\chi \rightarrow \infty$. For perturbative interaction strengths $\delta \ll 1$ this regime is defined by

$$\chi > \chi_{crit}(\delta) \equiv \sqrt[4]{\frac{243}{40}} \frac{1}{\delta^{\frac{3}{2}}}. \quad (3.42)$$

Using the concept of truncation one can execute a thorough and laborious pinning analysis which reveals the occurrence of quasipinning in the truncated setting $\wedge^3[\mathcal{H}_1^{(10)}]$. The minimal distance as a function of δ and χ is computed as:

$$D_{min}(\delta, \chi) = \frac{4}{9\chi^4}\delta^2 + \frac{20}{2187}\delta^8 + \mathcal{O}(\delta^{10}). \quad (3.43)$$

The truncation error of this analysis (cf. Eq. (3.34)) is of the order $\mathcal{O}(\delta)^{10}$, which is negligible since $D_{min} \propto \delta^8$ to leading order.⁷

Furthermore, taking the limit $\chi \rightarrow \infty$ as a consistency check reveals that

$$\lim_{\chi \rightarrow \infty} D_{min}(\delta, \chi) = \frac{20}{2187}\delta^8 + \mathcal{O}(\delta^{10}), \quad (3.44)$$

which coincides with the quasipinning found for the strictly one-dimensional 3-Harmonium (see Eq. (16) in Ref. [87]).

The result (3.43) indicates that the strength of quasipinning in one-dimensional systems is only slightly reduced when a second spatial dimension is added. This however, is not too surprising since the addition of spatial dimensions, whose degrees of freedom are frozen, should not impose changes on any physical quantities.

3.5 Fully spin-polarised Harmonium in higher spatial dimensions

Having presented an analysis on quasipinning of the Harmonium ground state in quasi-one-dimensional setups in the previous section, we will now consider an extension to higher spatial dimensions assuming a complete alignment of all spins, i.e. freezing out the spin degree of freedom.

3.5.1 Two spatial dimensions and corresponding dimensional crossovers

To begin with, we consider the weak-coupling regime and restrict our analysis to the setup of an isotropic external trapping potential, i.e. $\omega^{(2)} = \omega^{(1)}$. This implies that

⁷By invoking condition (3.42), one gets $\delta^8 \gtrsim \delta^2/\chi^4$ which confirms δ^8 to be the leading order of D_{min} .

a single parameter suffices to describe the interaction strength (cf. Eqs. (3.12) and (3.26)), and so we set $\kappa \equiv \kappa^{(1)} = \kappa^{(2)}$ and $\delta \equiv \delta^{(1)} = \delta^{(2)}$, respectively. Because of the duality relation (3.27) it again proves helpful to compute the perturbative expansion series of the NONs in the interaction strength parameter δ . First, we discuss the case of three fermions. By invoking Thm. 3, one finds a unique Harmonium ground state with configuration $\mathcal{C} = \{\{0, 0\}, \{1, 0\}, \{0, 1\}\}$. Up to corrections of the order $\mathcal{O}(\delta^8)$, the corresponding NONs read:

$$\begin{aligned}
\lambda_1(\delta) &= 1 - \frac{32\delta^4}{81} + \frac{224\delta^6}{729} + \mathcal{O}(\delta^8), \\
\lambda_2(\delta) &= \lambda_3(\delta) = 1 - \frac{4\delta^2}{9} + \frac{4\delta^4}{27} - \frac{152\delta^6}{3645} + \mathcal{O}(\delta^8), \\
\lambda_4(\delta) &= \lambda_5(\delta) = \frac{4\delta^2}{9} - \frac{8\delta^4}{27} + \frac{16\delta^6}{135} + \mathcal{O}(\delta^8), \\
\lambda_6(\delta) &= \lambda_7(\delta) = \frac{4\delta^4}{27} - \frac{88\delta^6}{729} + \mathcal{O}(\delta^8), \\
\lambda_8(\delta) &= \lambda_9(\delta) = \frac{4\delta^4}{27} - \frac{40\delta^6}{243} + \mathcal{O}(\delta^8), \\
\lambda_{10}(\delta) &= \frac{8\delta^4}{81} - \frac{16\delta^6}{243} + \mathcal{O}(\delta^8), \\
\lambda_{i \geq 11}(\delta) &= \mathcal{O}(\delta^6).
\end{aligned} \tag{3.45}$$

Note that some NONs are degenerate in pairs. This is a direct consequence of the substructure of the 1-RDO as given by Eq. (3.25), since in the case of an isotropic trap $\text{spec}[\rho_{1,oe}^{(f)}] = \text{spec}[\rho_{1,eo}^{(f)}]$. It should also be stressed that the extension of the perturbation series to deformed anisotropic traps is a bit more tedious but can be accomplished in a similar fashion.

To determine the minimal distance of the $\vec{\lambda}$ -vector (3.45) to the boundary of the polytope, we again have to apply the concept of truncation. The analysis becomes conclusive in the truncated setting $\wedge^3[\mathcal{H}_1^{(10)}]$, where we find that

$$D_{\min}(\delta) = \frac{8}{27}\delta^4 + \mathcal{O}(\delta^6). \tag{3.46}$$

The leading order of the truncation error is determined by the leading order of the largest neglected NON, i.e. $\lambda_{11} \sim \mathcal{O}(\delta^6)$. It is smaller than $D_{\min}$ by two orders in δ .

The distance of the $\vec{\lambda}$ -vector (3.45) to the Hartree-Fock point (cf. Eq. (3.31)) is derived as

$$\text{dist}_1(\vec{\lambda}, \vec{\lambda}_{HF}) \equiv D_{HF}(\delta) = \frac{8}{9}\delta^2 + \frac{8}{81}\delta^4 + \mathcal{O}(\delta^6). \tag{3.47}$$

Note that it is larger than $D_{\min}$ by two orders in δ . In contrast to the minimal distance observed in one-dimensional Harmonium however ($D_{\min} \sim \delta^8$), this quasip-

(N, n)	$\mathcal{O}(\delta^2)$	$\mathcal{O}(\delta^4)$	$\mathcal{O}(\delta^6)$	D_{min}	10^{-Q}
$(3, 2)$	$\wedge^2[\mathcal{H}_1^{(4)}]$	$\wedge^3[\mathcal{H}_1^{(10)}]$	$\wedge^3[\mathcal{H}_1^{(14)}]$	$\propto \delta^4$	$\propto \delta^0$
$(4, 2)$	$\wedge^3[\mathcal{H}_1^{(7)}]$	$\wedge^4[\mathcal{H}_1^{(13)}]$	$\wedge^4[\mathcal{H}_1^{(20)}]$	$\propto \delta^4$	$\propto \delta^2$
$(5, 2)$	$\wedge^3[\mathcal{H}_1^{(7)}]$	$\wedge^5[\mathcal{H}_1^{(14)}]$	$\wedge^5[\mathcal{H}_1^{(20)}]$	$\propto \delta^4$	$\propto \delta^0$
$(6, 2)$	$\wedge^3[\mathcal{H}_1^{(7)}]$	$\wedge^5[\mathcal{H}_1^{(14)}]$	$\wedge^5[\mathcal{H}_1^{(21)}]$	$\propto \delta^6$	$\propto \delta^0$
$(7, 2)$	$\wedge^4[\mathcal{H}_1^{(9)}]$	$\wedge^6[\mathcal{H}_1^{(17)}]$	$\wedge^7[\mathcal{H}_1^{(24)}]$	$\propto \delta^6$	$\propto \delta^0$

Table 3.3: For the N -Harmonium ground states in $n = 2$ spatial dimensions we present the ‘active space structures’ by considering NONs with corrections to the values 1 or 0 up to the orders $\mathcal{O}(\delta^2)$, $\mathcal{O}(\delta^4)$ and $\mathcal{O}(\delta^6)$, respectively. The results on quasipinning are presented (D_{min}) as well as its ‘non-triviality’, quantified by the Q -parameter (see text).

inning effect is less pronounced. Here, we see a first indication that reduced spatial dimensionality might be essential for the occurrence of strong quasipinning.

Similar to the case of $N = 3$ particles, one can study the ground states of two-dimensional Harmonium for $N > 3$. We have computed the Taylor series expansions of the corresponding NONs for the cases $N = 4, 5, 6, 7$. The results are summarised in Tab. 3.3. From left to right the columns display the respective number of particles and spatial dimensions (N, n) , the active spaces $\wedge^{N'}[\mathcal{H}_1^{(d')}]$ on the order scales of δ^2 , δ^4 , δ^6 , the minimal distance to the polytope boundary and the Q -measure.

Let us specify the notion of the active space structure. On the scale of $\mathcal{O}(\delta^r)$, the active space structure $\wedge^{N'}[\mathcal{H}_1^{(d')}]$ is given by all N' NONs, $\lambda_{N-N'+1}, \dots, \lambda_N$, and all $d' - N'$ NONs, $\lambda_{N+1}, \dots, \lambda_{N+d'-N'}$, which have corrections on the scales δ^s , $s \leq r$ to the maximal values 1 and 0, respectively. The manifestation of active space structures is a remarkable property of the Harmonium model and can even be proven analytically. With respect to pinning analyses it provides a suitable means to determine the size of the truncated setting that is required to achieve a negligible error. The results of respective analyses are also shown in Tab. 3.3. For particle numbers $N = 4, 5$ the quasipinning strength is calculated as δ^4 and increases to δ^6 for $N = 6, 7$. As for one-dimensional Harmonium, adding particles to the system increases the quasipinning. This supports the notion of a ‘microscopic Pauli pressure’ mentioned earlier, which forces the $\vec{\lambda}$ -vector closer to the boundary of the polytope. We note that this pressure also relies on the active space structure, which, due to degenerate angular degrees of freedom, is less-pronounced for two-dimensional Harmonium than for its one-dimensional counterpart (cf. Tab. 3.1).

Recall that the inclusion relation $\mathcal{P} \subset \Sigma$ (cf. Fig. 2.1) implies that the minimal distance D_{min} is bounded from above by at least $1 - \lambda_1$, which is the distance to the $(\lambda_1 = 1)$ -facet of the Pauli simplex Σ . To examine the non-triviality of quasipinning in two-dimensional Harmonium, we evaluate the Q -measure at the Taylor series expansions of the respective NONs. A $\vec{\lambda}$ -vector with Q -value $Q(\vec{\lambda})$ lies $10^{Q(\vec{\lambda})}$ closer to the boundary of the polytope than could be expected from the saturation of Pauli's exclusion principle. The respective values for 10^{-Q} are displayed in the right column of Tab. 3.3. For all particle numbers except $N = 4$ the quasipinning is found to be trivial. For $N = 4$ particles, it is non-trivial by two orders in δ . A comparison with the results on the Q -measure in one-dimensional Harmonium (cf. Eq. (3.33)) suggests that GPCs are more relevant in lower-dimensional systems. In what follows, further evidence for this behaviour will be provided by studying dimensional crossovers of Harmonium systems. These crossovers are achieved by detuning one trapping frequency with respect to the other, thus causing the system to undergo a transition to the effectively one-dimensional regime.

Let us now consider three fermions in two spatial dimensions. Instead of (κ_1, κ_2) one can also use the parameters $\kappa \equiv \kappa_1$ and the frequency detuning $\chi \equiv \omega_2/\omega_1 \geq 1$ to characterise the coupling regime (recall Eq. (3.12)). For smaller detunings, the Harmonium ground state assumes the configuration $\boldsymbol{\mu} = \{\{0, 0\}, \{1, 0\}, \{0, 1\}\}$ (cf. Fig. 3.1). When χ is increased while keeping κ fixed, the configuration of boxes changes. As a result, at some specific critical value the ground state configuration becomes $\boldsymbol{\mu}' = \{\{0, 0\}, \{1, 0\}, \{2, 0\}\}$. The variation of χ thus induces a crossover from two to one spatial dimension (see also related discussion and remarks in Sec. 3.4). In the κ - χ parameter plane, the transition line between the two ground state configurations is given by

$$\kappa_{crit} = -\frac{4}{3} + \frac{1}{3}\chi^2. \quad (3.48)$$

To explore the behaviour of quasipinning over a range of parameters κ and χ , pinning analyses have been carried out at a number of logarithmically distributed data points in the κ - χ -plane. The required spectra were derived by numerical diagonalisation of analytically computed 1-RDOs. Thereafter, interpolation functions for $D_{min}(\kappa, \chi)$ and $Q(\kappa, \chi)$ have been determined by using the respective values at the data points. The results are presented in Fig. 3.5. Note that over the entire range of parameters considered, the truncation errors of the pinning analyses were found negligible.

Note also, that in Fig. 3.5 the solid line represents the transition line (3.48) between the configurations $\boldsymbol{\mu}$ and $\boldsymbol{\mu}'$. The dashed lines correspond to crossings of some of the

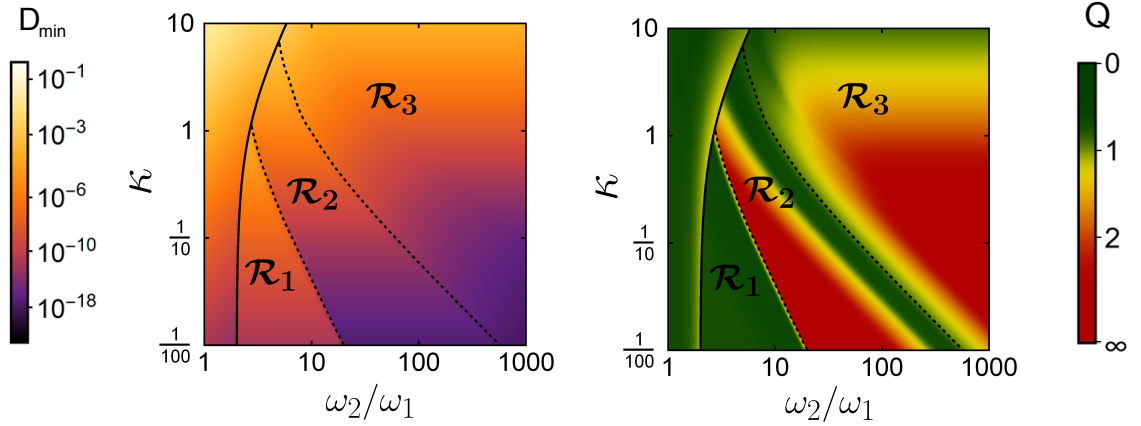


Figure 3.5: Quasipinning results for the 3-Harmonium ground state in two spatial dimensions with external trap frequencies ω_1, ω_2 and coupling strength κ . Minimal distance D_{min} of $\vec{\lambda}$ to polytope boundary is shown on the left and its ‘non-triviality’ is quantified on the right. The solid line represents the boundary $\kappa_{crit}(\chi)$ in between the two different ground state configurations with the effectively one-dimensional one on the right. Dashed lines mark relevant crossing of NONs (see text for more details).

relevant NONs.⁸ These crossings and the associated re-orderings of NONs lead to structurally different behaviours of the quasipinning in the regimes $\mathcal{R}_i$.

In Fig. 3.5, we see that the minimal distance D_{min} decreases monotonically when the particle-particle interaction strength κ becomes smaller. This is not too unexpected since the $\vec{\lambda}$ -vector of systems with lower interaction strengths and thereby reduced correlations approaches the Hartree-Fock point. In the isotropic setting $\omega_1 = \omega_2$, the numerically determined minimal distances in Fig. 3.5 agree with the analytical perturbative expression for D_{min} derived above in Eq. (3.46), even up to $\kappa = 10$.⁹ One also recognises that D_{min} decreases when the trapping potential becomes narrower by increasing ω_2/ω_1 . This is another piece of evidence for the existence of the ‘microscopic Pauli pressure’ discussed in former sections. By constraining the particles within an effectively lower dimensional trapping potential, the number of available levels around the Fermi level is reduced which decreases the size of the active spaces. Interestingly, the state with configuration $\mu = \{\{0, 0\}, \{1, 0\}, \{0, 1\}\}$ (which for large detunings becomes an excited state) also exhibits stronger and stronger quasipinning when χ is increased.¹⁰

⁸The left dashed line describes $\lambda_4 = \lambda_5$ and the right one $\lambda_6 = \lambda_7$. Although further crossings of other NONs exist, the concept of truncation implies that these will not be of relevance to the value of the minimal distance.

⁹Recall that $\delta = 1$ translates into $\kappa \approx 55$ (cf. Eq. (3.26)).

¹⁰Of course, this is not shown in Fig. 3.5, where only the quasipinning of the ground state is displayed.

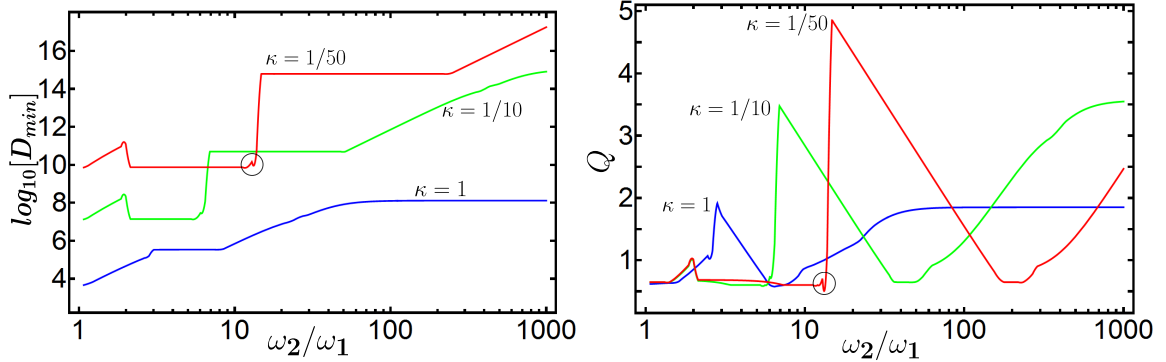


Figure 3.6: Left: Minimal distance D_{min} of $\vec{\lambda}$ to the polytope boundary as a function of the trap frequency detuning $\chi \equiv \omega_2/\omega_1$ for fixed particle-particle interaction strengths κ . Right: Relevance of the quasipinning by GPCs beyond Pauli’s exclusion principle as measured by the Q -parameter.

The relevance of the quasipinning beyond the Pauli exclusion principle as measured by the Q -parameter, however, shows a more complex and different behaviour to D_{min} . For $\kappa \lesssim 1$ fixed, the system undergoes multiple changes from ‘trivial’ quasipinning (green) to highly ‘non-trivial’ quasipinning (red). Between different regimes $\mathcal{R}_i$ within the effectively one-dimensional state configuration, we observe sharp gradients in both, the Q -parameter as well as the minimal distance D_{min} . To study these transitions further, we consider fixed κ -sections in Fig. 3.6. Evidently, the absolute quasipinning is not strongly affected by the change of the ground state configuration. This is different at the first dashed line where $\lambda_4 = \lambda_5$. Over a short range of values ω_2/ω_1 the minimal distance increases by several orders in the sections with $\kappa = 1/10, 1/50$. At the same time, the character of this quasipinning changes from ‘trivial’ to highly ‘non-trivial’. Furthermore, we notice that the observed finer structure (see, e.g., the ‘black’ circles) has to be attributed to crossings of smaller eigenvalues which - as may be seen from the concept of truncation - does not severely affect the quasipinning behaviour.

The case of four particles in two spatial dimensions is comprised within the analysis of four particles in three spatial dimensions considered in the next section.

3.5.2 Three spatial dimensions and corresponding dimensional crossovers

Let us examine the regime of weak couplings $\delta \ll 1$ again. For the particle numbers $N = 3, 4, 5, 6$ the results of comprehensive pinning analyses for the three-dimensional Harmonium ground state in an isotropic trapping potential are shown in Tab. 3.4.

(N, n)	$\mathcal{O}(\delta^2)$	$\mathcal{O}(\delta^4)$	$\mathcal{O}(\delta^6)$	D_{min}	10^{-Q}
$(3, 3)$	$\wedge^3[\mathcal{H}_1^{(8)}]$	$\wedge^3[\mathcal{H}_1^{(18)}]$	$\wedge^3[\mathcal{H}_1^{(32)}]$	$\mathcal{O}(\delta^4)$	$\mathcal{O}(\delta^2)$
$(4, 3)$	$\wedge^3[\mathcal{H}_1^{(8)}]$	$\wedge^4[\mathcal{H}_1^{(20)}]$	$\wedge^4[\mathcal{H}_1^{(34)}]$	$\propto \delta^4$	$\propto \delta^0$
$(5, 3)$	$\wedge^4[\mathcal{H}_1^{(12)}]$	$\wedge^5[\mathcal{H}_1^{(26)}]$	$\wedge^5[\mathcal{H}_1^{(45)}]$	$\mathcal{O}(\delta^4)$	?
$(6, 3)$	$\wedge^5[\mathcal{H}_1^{(14)}]$	$\wedge^6[\mathcal{H}_1^{(29)}]$	$\wedge^5[\mathcal{H}_1^{(49)}]$	$\mathcal{O}(\delta^4)$	?

Table 3.4: For the N -Harmonium ground states in $n = 3$ spatial dimensions we present the ‘active space structures’ by considering NONs with corrections to the values 1 or 0 up to the orders $\mathcal{O}(\delta^2)$, $\mathcal{O}(\delta^4)$ and $\mathcal{O}(\delta^6)$, respectively. The results on quasipinning are presented (D_{min}) as well as its ‘non-triviality’, quantified by the Q -parameter. A question mark indicates that no analysis was possible due to too large active spaces.

Analogously to the case of two-dimensional Harmonium (cf. Tab. 3.3), the second, third and fourth columns display the active space structures attributed to the orders $\mathcal{O}(\delta^2)$, $\mathcal{O}(\delta^4)$ and $\mathcal{O}(\delta^6)$, respectively. One recognises that the additional angular degrees of freedom in three-Harmonium give rise to significantly enlarged dimensions of the active spaces. This in turn is found to decrease the ‘Pauli pressure’. Due to the lack of knowledge about the specific form of the GPCs for one-particle Hilbert space dimensions greater than 11,¹¹ the increased dimensions of the active spaces prevent the execution of a *conclusive* quasipinning analysis for all cases but $N = 4$. This is also indicated in the right two columns of Fig. 3.4. To perform an analysis for particle numbers $N = 5, 6$ one at least needs to know the GPCs of the settings $(N, d) = (4, 12)$ and $(5, 14)$, respectively. A lower bound on the strength of quasipinning for these particle numbers can be derived by invoking the inclusion relation $\mathcal{P} \subset \Sigma$, which implies that $D_{min} < 1 - \lambda_1$ is at least of fourth order in δ . For $N = 3$ particles, the pinning analysis is not conclusive since the truncation error is of fourth order, too. Note that only for $N = 3$ particles the Q -measure indicates non-trivial quasipinning by two orders in δ .

To investigate anisotropic systems and gain more understanding about the influence of the spatial dimension on the quasipinning effect, we shall now consider dimensional crossovers in a system with four fermions. Again we set $\kappa \equiv \kappa_1$ and use the detuning parameters $\chi_1 = \omega_2/\omega_1$ and $\chi_2 = \omega_3/\omega_1$ to describe the coupling regime. The results are shown in Fig. 3.7. From left to right we start with an isotropic potential, i.e. $\omega_1 = \omega_2 = \omega_3$, and detune ω_3 while keeping ω_2 constant. Once $\omega_3 = 1000\omega_1$

¹¹See remarks in Sec. 2 on the complexity of deriving GPCs for arbitrary settings (N, d) .

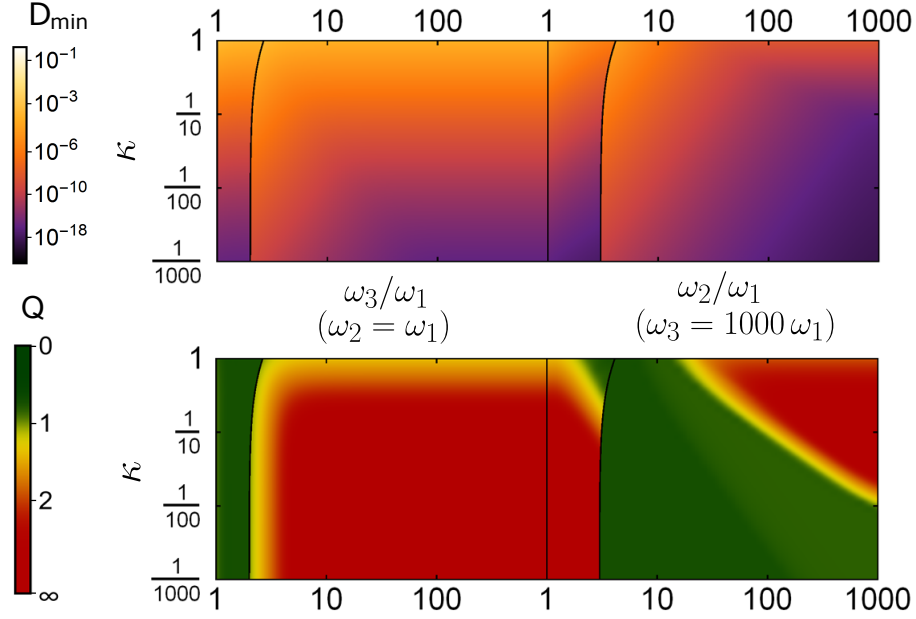


Figure 3.7: Quasipinning results for the 4-Harmonium ground state in three dimensions with external trap frequencies $\omega_1, \omega_2, \omega_3$ and coupling strength κ . Minimal distance D_{min} of $\vec{\lambda}$ to polytope boundary is shown in the upper diagram and its ‘non-triviality’ Q is quantified in the lower diagram (see text for details). The left and right solid curve indicate a change of the ground state configuration.

we keep ω_3 constant and also ramp up ω_2 to $1000\omega_1$. Initially, the system has a ground state configuration of $\boldsymbol{\mu} = \{\{0, 0, 0\}, \{1, 0, 0\}, \{0, 1, 0\}, \{0, 0, 1\}\}$. When χ_2 is increased this changes to the configuration $\boldsymbol{\mu}' = \{\{0, 0, 0\}, \{1, 0, 0\}, \{0, 1, 0\}, \{2, 0, 0\}\}$ at the first solid line. The transition to the quasi-one-dimensional configuration $\boldsymbol{\mu}'' = \{\{0, 0, 0\}, \{1, 0, 0\}, \{2, 0, 0\}, \{3, 0, 0\}\}$ is achieved when χ_1 is also increased (second solid line). Note that κ has been restricted to the interval $[0, 1]$ to guarantee a sufficiently small truncation error. The range of κ values is seen to be reduced in comparison to the investigations on two-dimensional Harmonium (cf. Fig. 3.5). The necessity for this restriction originates in the larger dimensions of the active spaces in three-dimensional Harmonium.

From Fig. 3.7 we find that the minimal distance D_{min} of the $\vec{\lambda}$ -vector to the polytope boundary monotonically decreases with decreasing κ . Within each regime of state configuration $\boldsymbol{\mu}$, $\boldsymbol{\mu}'$ and $\boldsymbol{\mu}''$, the quasipinning becomes stronger with increased anisotropy of the trapping potential. A bit surprisingly, however, this does not hold at the respective boundaries (marked by solid curved lines), where the quasipinning strength falls sharply by several orders of magnitude. Recall that this has not been

observed at the dimensional crossover of $N = 3$ particles in two-dimensional Harmonium (see Figure 3.5).

The most striking aspect of the quasipinning analysis of this system, however, is revealed by a comparison of D_{min} and Q in the effectively one-dimensional configuration. While D_{min} decreases with smaller κ and larger ω_2/ω_1 , the Q -parameter shows that the quasipinning becomes ‘trivial’ in parameter regions with small D_{min} (c.f. lower right corner of the diagram) and that it becomes highly ‘non-trivial’ in parameter regions with large D_{min} (c.f. upper right corner of the diagram). This strongly demonstrates the importance of quantifying quasipinning by GPCs *beyond* quasipinning by Pauli exclusion principle constraints.

Let us add a closing remark on degeneracies of the eigenspaces of Harmonium in higher dimensions. The ‘box picture’ (see Fig. 3.1) reveals the occurrence of shell structures in Harmonium systems, where an additional rotational symmetry is given whenever two or more trapping frequencies will be equal. For example, $N = 4$ particles in two dimensional Harmonium with $\omega_1 = \omega_2$ will have a three-fold degenerate ground state space. The obvious question whether superpositions of these states may experience a different quasipinning has been addressed by considering various superpositions, including the rotational symmetry adapted eigenstates. The quasipinning behaviour of these states was found to show the same scaling as the one for non-symmetry adapted states. Hence, they have not been displayed separately in the Tables 3.3 and 3.4.

3.6 Spinful Harmonium

So far, the quasipinning effect has been studied for spinless or fully polarised fermions. In the present section, the spin degree of freedom shall eventually be taken into account which brings a number of challenges. First, each spatial orbital splits into $2S + 1$ levels, where S denotes the spin of the particles. By increasing the dimensions of the active spaces, this causes a reduction of the Pauli pressure and might thus decrease the relevance of GPCs as well. Moreover, the additional spin degrees of freedom will make an interpretation more involved. A finite degree of polarisation, however, will allow us to consider changes of the quantum state which are induced by a variation of the external magnetic field. The development of these conceptual ideas might further be useful in finding a way for the experimental realisation of the quasipinning phenomenon (cf. discussion in chapter 5).

In the following, we shall focus on spin- $\frac{1}{2}$ fermions, which requires an extension of the N -particle Hilbert space to $\wedge^N[L_2[\mathbb{R}^n] \otimes \mathbb{C}^2]$. The spins shall be coupled to an external homogenous magnetic field $\vec{B}$ via an additional Zeeman interaction term $\hat{H}_Z = -c\hbar \sum_{i=1}^N \vec{s}_i \cdot \vec{B}$ in the Hamiltonian (3.1). Here, c denotes a coupling constant.¹²

The Zeeman term commutes with the spatial part of the Hamiltonian (3.1), which allows us to adopt the ‘box’ picture to the case of spinful fermions. We replace each orbital $\phi_{\mu_j}^{(i)}(\vec{x}_j)$ in the Slater determinant of Eq. (3.5) by the product state of ϕ with a spin state $|\sigma_j\rangle \in \{|\uparrow\rangle, |\downarrow\rangle\}$. Note that the spin states have been defined with respect to the quantisation axis $\vec{B}/B$. As a consequence of the level splitting due to the additional spin degree of freedom, *two* ‘box arrays’ associated with $|\uparrow\rangle$ and $|\downarrow\rangle$ arise. Their respective boxes are energetically separated by $\langle\downarrow|\hat{H}_Z|\downarrow\rangle - \langle\uparrow|\hat{H}_Z|\uparrow\rangle = c\hbar|B|$. The ground state configuration $\bar{\mu} = (\mu^\uparrow, \mu^\downarrow)$ may now be derived by distributing N particles on the N energetically lowest levels. The form of the ground state wave function is given by the modified version of Eq. (3.5). Let us consider the example of $N = 4$ particles in an isotropic two-dimensional trapping potential of frequency $\omega_1 = \omega_2 \equiv \omega$. If the external magnetic field suffices $\omega\sqrt{1+\kappa}/c < |B| < 2\omega\sqrt{1+\kappa}/c$, then the ground state configuration becomes $\mu^\downarrow = \{\{0, 0\}, \{1, 0\}, \{0, 1\}\}$ and $\mu^\uparrow = \{\{0, 0\}\}$.

At first, we consider one-dimensional Harmonium in the weak coupling regime $\delta \ll 1$ with $N = 3, 4$ spinful fermions. Depending on the magnitude of the external magnetic field B and the interaction strength δ , there are a couple of different ground states which can be characterised by their magnetic quantum number M . For $N = 3$ we have $M = \pm\frac{3}{2}, \pm\frac{1}{2}$ and for $N = 4$ the magnetic quantum number can assume the values $M = \pm 2, \pm 1, 0$. By performing conclusive pinning analyses for all these states, one gets

$$D_{min}(\delta) \sim \delta^{4+2|M|}. \quad (3.49)$$

Observe that the strength of the quasipinning strongly increases with the degree of spin polarisation. Once again, this is an indicator for the proposed notion of a microscopic Pauli pressure originating in the structure of the active spaces. By increasing the degree of polarisation, the conflict between energy minimisation and the antisymmetry intensifies which in turn leads to stronger quasipinning.

To characterise the relevance of this quasipinning of GPCs one has to invoke the Q -measure. For $N = 3$ the quasipinning is non-trivial by two orders in δ for all values of the magnetic quantum number, $|M| = \frac{3}{2}, \frac{1}{2}$. For $N = 4$ however, this only

¹²We skip the coupling of the magnetic field to the angular momentum of the fermions by assuming them to be uncharged. One could in principle extend our model to charged fermions which, however, would significantly complicate the description of the ground state for non-isotropic traps.

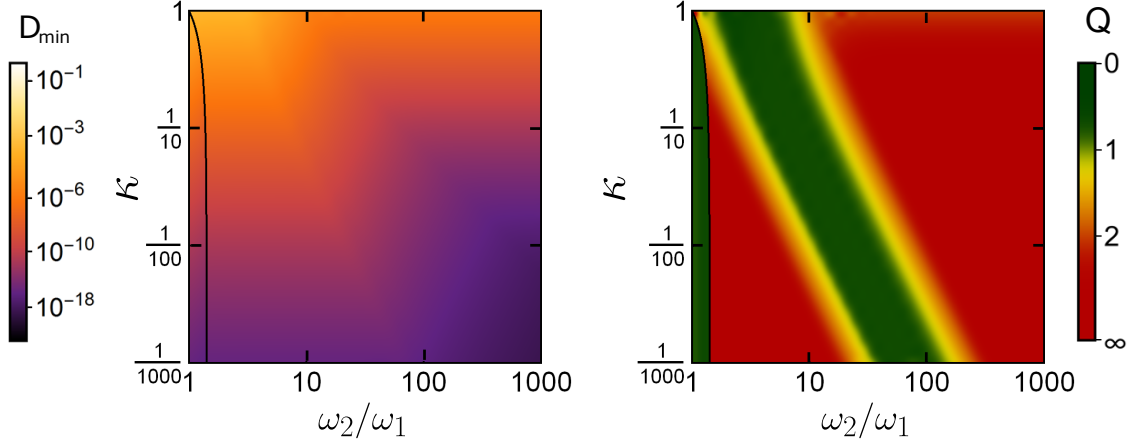


Figure 3.8: Quasipinning results for the non-fully spin-polarised 3-Harmonium ground state in two spatial dimensions with external trap frequencies ω_1, ω_2 , coupling strength κ and some fixed homogenous magnetic field B fulfilling $\omega\sqrt{1+\kappa} < c|B| < 2\omega\sqrt{1+\kappa}$. Minimal distance D_{min} of $\vec{\lambda}$ to polytope boundary is shown in the left diagram and its ‘non-triviality’ is quantified in the right diagram by the Q -parameter. The solid line marks the boundary between the effective two- and one-dimensional ground state configurations.

holds true for full polarisation, $|M| = 2$.¹³ For $|M| = 0, 1$ the quasipinning becomes trivial. Especially for $|M| = 0$, this is not surprising since the ground state becomes a spin-singlet state for which the only constraints on the NONs are given by the Pauli exclusion principle constraints (cf. Ref. [88]).

Finally, we explore the influence of dimensionality on spinful Harmonium by considering three fermions in two spatial dimensions. The coupling regime can be characterised by the parameters $\kappa \equiv \kappa_1$ and $\chi = \omega_2/\omega_1$ (cf. related remarks in the previous section). The trap may initially be isotropic, i.e. $\chi = 1$, and the magnetic field strength may be chosen such that $\omega\sqrt{1+\kappa} < c|B| < 2\omega\sqrt{1+\kappa}$. Consequently, the ground state configuration is given by the index sets $\boldsymbol{\mu}^\uparrow = \{\{0, 0\}, \{1, 0\}, \{0, 1\}\}$ and $\boldsymbol{\mu}^\downarrow = \emptyset$. By narrowing the trap, i.e. increasing χ , a dimensional crossover will be induced and the new quasi-one-dimensional ground state configuration becomes $\boldsymbol{\mu}^\uparrow = \{\{0, 0\}, \{0, 1\}\}$ and $\boldsymbol{\mu}^\downarrow = \{\{0, 0\}\}$. Similar to the investigations in Sec. 3.5, pinning analyses have been carried out for a number of logarithmically distributed points in the κ - χ -parameter plane. The interpolated results are shown in Fig. 3.8.

Whereas the minimal distance D_{min} of $\vec{\lambda}$ to the polytope boundary becomes smaller when reducing κ and increasing $\chi = \omega_2/\omega_1$, the behaviour of the Q -parameter

¹³Note that the fully-polarised Harmonium retrieves the system of spinless fermions studied before (cf. Sec. 3.3).

is more complex and shows similarities to the fully spin-polarised case in Section 3.5. Again, the crossing of NONs induces different regimes leading to a high-low-high transition of the Q -values when increasing χ for a fixed interaction strength κ . This once more demonstrates the significance of the Q -parameter as it unveils the importance of GPCs beyond the Pauli exclusion principle in parameter ranges with attributed moderate minimal distances D_{min} . Last but not least, in the regime of the two-dimensional ground state configuration, i.e. left to the solid black line, the quasipinning is ‘trivial’ (‘green’).

Chapter 4

The 1-body N -representability problem for hardcore bosons

In the previous part, the scope and influence of the fermionic exchange statistics in form of the GPCs have been thoroughly studied. Generally, bosonic and fermionic particle statistics are known to be at the heart of dramatically different behaviours of their respective sorts of matter. This opens the question whether it might be possible to interpolate between the two particle species in order to gain more understanding about the specific character of the constraining mechanisms in fermionic statistics.

Good candidates for such an endeavour are hardcore bosons. Similar to fermions, they obey a form of a basis dependent exclusion principle which originates in a large repulsive particle-particle interaction. Yet they also exhibit bosonic statistics. The concepts and notion of hardcore bosons arise in the context of the Hubbard model and have seen application in a variety of disciplines beyond their well-known usage in condensed matter and atomic physics. Amongst others these are emergent gravity scenarios (see, e.g., Refs. [55, 54, 39, 17, 16, 37]), the study of chemical reactions (see, e.g., Refs. [46, 74, 71]) and biological processes (see, e.g., Refs. [5, 90]).

In the treatment of fermions we have seen that the indistinguishability of particles allows one to efficiently¹ describe a plethora of physical properties by invoking the concept of reduced particle information. Notably, this holds for the energy expectation value which, for physical fermionic Hamiltonians, comprising only 1-body and 2-body terms, becomes a functional of the 2-RDO (cf. Eq. (2.25)). By the form of this functional the Hamiltonian may be regarded as a flow vector field and gives rise to equi-energy hyperplanes in the space of two-particle density operators. Since the set

¹Efficiently in this context refers to polynomial scaling of the required information (cf. discussion at the end of Sec. 2.2).

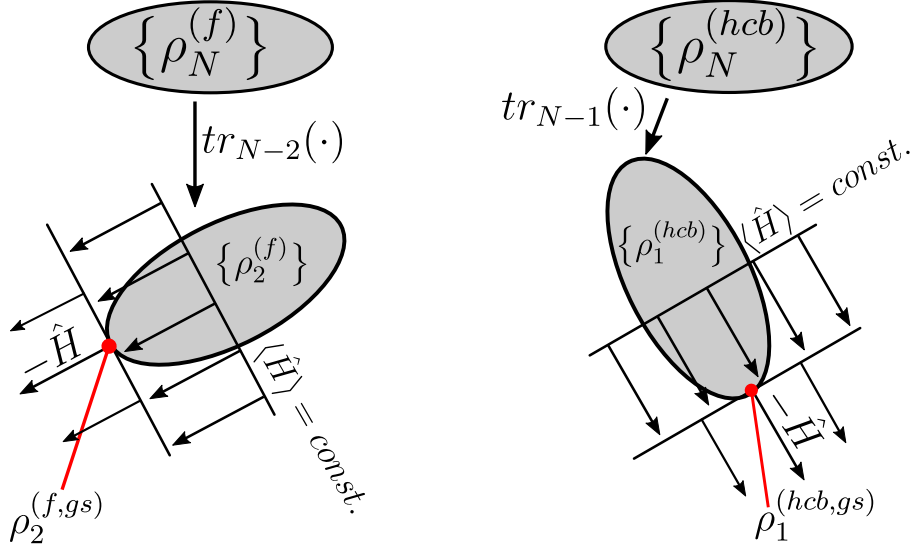


Figure 4.1: Illustration of the Hamiltonian flow $-\hat{H}$ on the 2-RDO and 1-RDO spaces of fermions $\{\rho_2^{(f)}\}$ (left), and hardcore bosons $\{\rho_1^{(hcb)}\}$ (right), respectively. Equi-energy hypersurfaces are orthogonal to the Hamiltonian flow and give rise to the position of the ground state reduced density operators $\rho_2^{(f,gs)}$ and $\rho_1^{(hcb,gs)}$ on the boundaries. For more details see text.

of compatible 2-RDOs is convex, the ground state energy is attained on its boundary. An illustration of this concept is drawn on the left of Fig. 4.1.

The entire concept of reduced particle information may also be translated to systems of hardcore bosons. If further the 2-body interaction terms of a particular system should only be given by the terms of the on-site hardcore interaction (a concise definition and treatment will shortly be given in Sec. 4.1), then the *one*-particle information is already sufficient to determine the ground state energy and other properties. A schematic drawing is depicted on the right of Fig. 4.1. This especially implies that an efficient description of the set of compatible hardcore boson 1-RDOs will allow for an efficient treatment of the underlying many-body dynamics.

In this part of the thesis, results of investigations on the 1-body N -representability problem for hardcore bosons and related questions shall be presented. To begin with, notations and conventions will be defined in Sec. 4.1. The sets of compatible one-particle spectra of hardcore bosons are different to those of common bosons and fermions. In Sec. 4.2 this fact will be demonstrated with the aid of an example. Despite permitting at most one particle on a spatial orbital, hardcore bosons will be found to populate some natural orbitals in numbers larger than one. In Sec. 4.3, a key theorem on the upper bound of hardcore boson NONs will be proven. For N

particles on d one-particle levels this bound will be determined as:

$$\lambda_{max} = \frac{N}{d}(d - N + 1). \quad (4.1)$$

Additionally, the structure of the states which saturate λ_{max} will be examined in detail.

In Sec. 4.4, a scheme will be presented which allows one to derive necessary conditions for the 1-body N -representability of hardcore bosons. The key idea will be to use concepts of constrained optimisation to evaluate the upper and lower bounds of $\text{tr}(\rho_1^m)$. This in turn will impose restrictions on the $\vec{\lambda}$ -vector. Furthermore, the extension to sets of necessary and sufficient conditions will be studied.

In the next section, bounds on one-particle entropy measures of hardcore bosons will be determined and compared with their counterparts of common bosons and fermions. The results will provide strong testimony of the hybrid character of hardcore bosons: for smaller systems, hardcore bosons are found to behave like fermions, whereas for an increasing number of levels, they become boson-like in the thermodynamic limit.

In Sec. 4.6, examples will be given of hardcore boson states whose $\vec{\lambda}$ -vectors are exactly pinned to the boundary of the set of compatible spectra. More specifically, the considered physical systems will allow one to engineer the occupation number maximising state.

A discussion and outlook will be provided in the next chapter.

4.1 Exposition

To begin with, we provide a rigorous definition of hardcore bosons and present their major properties. Consider N bosons in a system with a d -dimensional underlying one-particle Hilbert space $\mathcal{H}_1^{(d)}$. The associated N -particle Hilbert space $\mathcal{H}_N^{(d)}$ (2.6) and the language of second quantisation have been introduced in the first chapter. Assume that a specific one-particle basis of $\mathcal{H}_1^{(d)}$ is distinguished by physical means. Although this can most prominently be realised by systems of ultracold bosonic atoms in optical lattices [58, 59], other mechanisms and systems are conceivable as well (see, e.g., Refs. [91, 35, 92, 41]). The selected physical one-particle basis shall be called the *hardcore boson, lattice* or simply *hardcore* basis $\mathcal{B}_{hcb}$.

$$\mathcal{B}_{hcb} := \{|i\rangle\}_{i=1}^d. \quad (4.2)$$

General physical Hamiltonians of N -boson systems comprise of 1- and 2-body terms² (2.24) from which one can extract the lattice related on-site interaction $\hat{H}_{hcb}$:

$$\hat{H} = - \sum_{i,j=1}^d (t_{ij} \hat{b}_i^\dagger \hat{b}_j + h.c.) - \sum_{\substack{i_1, \dots, i_4=1 \\ i_l \neq i_{l+1}}}^d (V_{i_1 i_2 i_3 i_4} \hat{b}_{i_1}^\dagger \hat{b}_{i_2}^\dagger \hat{b}_{i_3} \hat{b}_{i_4} + h.c.) + \underbrace{\frac{U_0}{2} \sum_i (\hat{b}_i^\dagger \hat{b}_i (\hat{b}_i^\dagger \hat{b}_i - 1))}_{\equiv \hat{H}_{hcb}}. \quad (4.3)$$

Note that the ladder operators are defined with respect to the lattice basis $\mathcal{B}_{hcb}$.

For large repulsive interaction strength U_0 , the bosons become impenetrable. N -boson states are called *hardcore boson* states if the expectation value of $\hat{H}_{hcb}$ vanishes:

$$\rho_N, |\psi_N\rangle \text{ hardcore} \iff \langle \hat{H}_{hcb} \rangle = 0. \quad (4.4)$$

This imposes an exclusion principle on the lattice site occupation numbers:

$$0 \leq \langle \hat{n}_i \rangle = \langle (\hat{b}_{|i\rangle})^\dagger \hat{b}_{|i\rangle} \rangle \leq 1, \quad \forall i = 1 \dots d. \quad (4.5)$$

Although there is a resemblance to the form of the Pauli exclusion principle for fermions, Eq. (2.27), these inequalities only hold in the particular lattice basis. In comparison to fermions, this gives rise to the distinct character of hardcore bosons.

Pure hardcore boson states can be expanded in terms of N -permanents of the lattice basis:

$$|\psi_N\rangle = \sum_{j_l < j_{l+1}}^d z_{j_1, j_2, \dots, j_N} |j_1, \dots, j_N\rangle \equiv \sum_{\mathbf{j} \in \mathbb{P}_N^d} z_{\mathbf{j}} |\mathbf{j}\rangle. \quad (4.6)$$

Since the space of mixed N -boson states $\mathcal{M}_N^{(b)}$ (2.8) is the convex hull of the pure N -boson states and since $\hat{H}_{hcb}$ is positive semi-definite, every mixed hardcore boson state can be written as a convex sum of pure hardcore boson states. This also implies that all r -particle reduced density operators of mixed hardcore boson states can be convexly decomposed in terms of r -particle reduced density operators of pure states.

$$\rho_r^{(mixed)} = \sum_i p_i \rho_r^{(pure), i}, \quad p_i \geq 0 \text{ and } \sum_i p_i = 1, \quad \forall r = 1 \dots N. \quad (4.7)$$

For a given hardcore basis $\mathcal{B}_{hcb}$ define the projectors $\hat{K}_N$ and $\hat{K}$ via

$$\hat{K}_N := \sum_{\mathbf{i} \in \mathbb{P}_N^d} |\mathbf{i}\rangle \langle \mathbf{i}|, \quad \hat{K} := \bigoplus_{N=1}^d \hat{K}_N. \quad (4.8)$$

²For instance, if one assumes that the particle-particle potential is given by a function of the particle positions only, $f(\hat{x}_1, \hat{x}_2)$, then the matrix elements V become: $V_{q_1, q_2; q'_1, q'_2} = \delta_{q_1, q'_1} \delta_{q_2, q'_2} f(q_1, q_2)$.

$\hat{K}_N$ acts on the N -bosonic Hilbert space $\mathcal{H}_N^{(b)}$ and $\hat{K}$ acts on the Fock space $\mathcal{F}^{(b)}$. Hardcore boson states span a linear subspace of the common boson state space. This allows one to consider the dynamical constraint imposed by $\hat{H}_{hcb}$ as a kinematical constraint and restrict the description of states and unitary evolution to the hardcore boson Hilbert space $\mathcal{H}_N^{(hcb)}$.

$$\mathcal{H}_N^{(hcb)} := \hat{K}_N \mathcal{H}_N^{(b)} \equiv \text{span}(|j_1, \dots, j_N\rangle \in \mathcal{H}_N^{(b)} | j_l < j_{l+1}) \leq \mathcal{H}_N^{(b)}. \quad (4.9)$$

In addition, the space of mixed N -hardcore boson states $\mathcal{M}_N^{(hcb)}$ is defined via:

$$\mathcal{M}_N^{(hcb)} := \hat{K}_N \mathcal{M}_N^{(b)} \hat{K}_N \leq \mathcal{M}_N^{(b)}. \quad (4.10)$$

Generally, the projection of $\mathcal{H}_N^{(b)}$ onto $\mathcal{H}_N^{(hcb)}$ induces a projection on the space of linear operators on $\mathcal{H}_N^{(b)}$. Observe that under this projection the $\hat{H}_{hcb}$ term in the general Hamiltonian (4.3) will be removed.

In analogy to fermions (cf. Def. 1) one can define the N -representability problem for hardcore bosons. In the following sections, we are now going to present results of investigations on the role and character of reduced-particle information in systems of hardcore bosons.

4.2 Hardcore bosons versus fermions: An illustrative example of 2 particles on 3 sites

Despite sharing some resemblance with respect to the exclusion principle on the lattice basis, the sets of N -representable one-particle density operators of hardcore bosons and fermions are quite different. In particular, one finds that, contrary to popular opinion, the natural occupation numbers of hardcore boson states can be larger than one. In order to get a first impression of the distinct one-particle nature of both particle species it is instructive to consider the example of two particles on three lattice sites. For common bosons, the set of allowed one-particle spectra is only constrained by the normalisation and ordering conditions, and the upper bound on each natural occupation number by $N = 2$. For pure fermionic states, however, we know that only the $\vec{\lambda}$ -vector $\vec{\lambda} = (1, 1, 0)$ is N -representable (cf. appendix, Sec. A). Remarkably, the hardcore boson constraint will yield yet another different set of N -representable one-particle spectra.

For $N = 2$ hardcore bosons on the $d = 3$ lattice sites, a normalised arbitrary pure state can be expressed in terms of the lattice basis $\{|1\rangle, |2\rangle, |3\rangle\}$ via

$$|\psi_{N=2,d=3}\rangle = z_1 |1, 2\rangle + z_2 |1, 3\rangle + z_3 |2, 3\rangle. \quad (4.11)$$

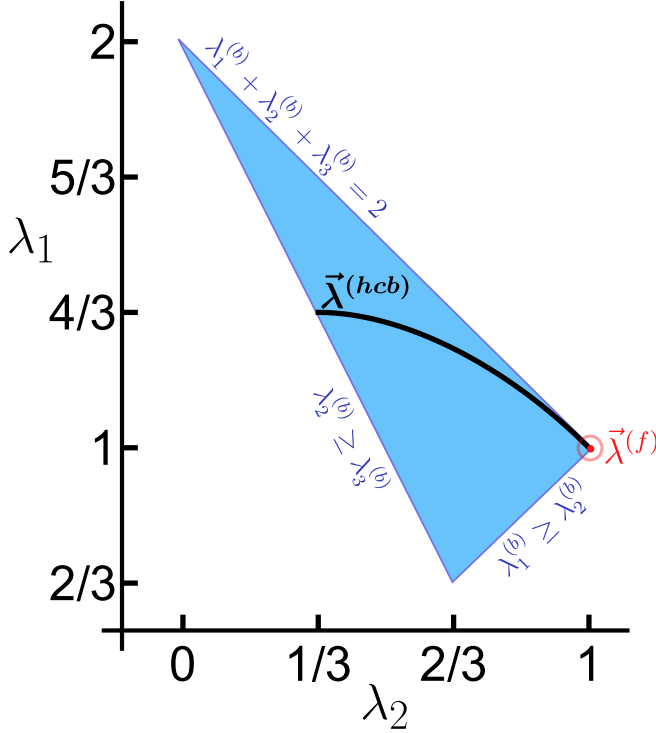


Figure 4.2: Pure N -representable one-particle reduced density operator spectra for systems of either $N = 2$ bosons (blue triangle), fermions (red dot at $(1, 1)$) or hardcore bosons (solid black line) on $d = 3$ lattice sites. The sets of spectra can be displayed in the (λ_1, λ_2) -plane since λ_3 is determined by the normalisation condition (see text for more details).

Normalisation to unity requires $\sum_i |z_i|^2 = 1$. In the lattice basis, the components of the one-particle reduced density matrix read³

$$\rho_{ij} \equiv (\langle i | \rho_1 | j \rangle)_{ij} = \begin{pmatrix} z_1 z_1^* + z_2 z_2^* & z_2 z_3^* & z_1 z_3^* \\ z_3 z_2^* & z_1 z_1^* + z_3 z_3^* & z_1 z_2^* \\ z_3 z_1^* & z_2 z_1^* & z_2 z_2^* + z_3 z_3^* \end{pmatrix}_{ij}. \quad (4.12)$$

In order to determine the set of compatible spectra, we consider the characteristic polynomial p_{ρ_1} of ρ_1 :

$$\begin{aligned} p_{\rho_1}(\lambda) &= \lambda^3 - 2(|z_1|^2 + |z_2|^2 + |z_3|^2) \lambda^2 + (|z_1|^2 + |z_2|^2 + |z_3|^2)^2 \lambda - 4|z_1|^2 |z_2|^2 |z_3|^2 \\ &= \lambda^3 - 2\lambda^2 + 1\lambda - c_0. \end{aligned} \quad (4.13)$$

In the second line, the polynomial has been simplified by using the normalisation condition of the wave function and defining $c_0 = 4|z_1|^2 |z_2|^2 |z_3|^2$. Regarded as a function on a compact domain, $c_0(\{z_i\}) : ([0, 1] \times [0, 2\pi])^3 \rightarrow 4|z_1|^2 |z_2|^2 |z_3|^2$, the λ^0 coefficient of the characteristic polynomial can be shown to lie within a compact interval, $c_0 \in [0, 4/27]$. The set of corresponding zero points $\{\lambda_i\}_{i=1}^3$ of $p_{\rho_1}|_{c_0}$ thus

³Note that the analogous fermionic 1-RDO differs from the hardcore boson 1-RDO by specific minus-signs: $\rho_1^{(f)} = \begin{pmatrix} z_1 z_1^* + z_2 z_2^* & z_2 z_3^* & -z_1 z_3^* \\ z_3 z_2^* & z_1 z_1^* + z_3 z_3^* & z_1 z_2^* \\ -z_3 z_1^* & z_2 z_1^* & z_2 z_2^* + z_3 z_3^* \end{pmatrix}$.

constitutes the set $\mathcal{C}^{(N=2,d=3)}$ of spectra of N -representable hardcore boson 1-RDOs. Due to the normalisation condition $\lambda_1 + \lambda_2 + \lambda_3 = 2$, it can readily be displayed in the (λ_1, λ_2) -plane, cf. Fig. 4.2. Note that in accordance with previous chapters the spectra will generally be ordered non-increasingly.

As expected, the set of compatible hardcore boson spectra, represented by the black solid line, forms a proper subset of the compatible spectra of common bosons, marked by the blue triangle. The only compatible fermionic spectrum $\vec{\lambda}^{(f)} = (1, 1, 0)$ is highlighted by a red dot. One observes, that unlike for fermions, the set $\mathcal{C}^{(2,3)}$ is not a polytope and does not even form a convex set. This suggests that the general description of 1-body N -representability conditions for pure hardcore boson states may be more intricate than its fermionic counterpart in terms of GPCs (cf. Sec. 2.3). For instance, an analogue of the fermionic particle-hole duality (see Eq. (2.32)) does not exist for $\mathcal{C}^{(2,3)}$ because this set is not isomorphic to the zero-dimensional set $\mathcal{C}^{(1,3)}$ obtained for a system of $N = 3 - 2 = 1$ particle(s) on 3 sites.

Last but not least, the set $\mathcal{C}^{(2,3)}$ in Fig. 4.2 also demonstrates that occupation numbers of one-particle states other than the lattice basis states are not restricted by the exclusion principle (4.5). In particular natural occupation numbers seem to have different upper bounds.

4.3 Maximal occupation numbers

Above we have seen that occupation numbers of hardcore boson states may well exceed the value of $\langle \hat{n} \rangle = 1$. This of course raises the question about the general form of an upper bound on the occupation numbers. In this section we are going to prove and discuss the following theorem:

Theorem 4 (Maximal hardcore boson occupation numbers)

Consider N hardcore bosons on d lattice sites with hardcore basis $\mathcal{B}_{hcb} \equiv \{|i\rangle\}_{i=1}^d$. The maximal possible occupation number λ_{max} ,

$$\lambda_{max} := \max_{\substack{|\phi\rangle \in \mathcal{H}_1^{(d)} \\ \rho_N \in \mathcal{M}_N^{(hcb)}}} \left(\text{tr}(\rho_N \hat{n}_{|\phi\rangle}) \right) = \frac{N}{d}(d - N + 1), \quad (4.14)$$

can be achieved for all $|\varphi\rangle \in \mathcal{H}_1^{(d)}$

$$|\varphi\rangle = \sum_{j=1}^d \frac{1}{\sqrt{d}} e^{i\phi_j} |j\rangle. \quad (4.15)$$

All other single particle states have always smaller occupation numbers.

The corresponding maximiser $|\psi_N^{\lambda_{max}}\rangle$ is a pure state and reads

$$|\psi_N^{\lambda_{max}}\rangle = \sum_{\mathbf{k} \in \mathbb{P}_N^d} \binom{d}{N}^{-\frac{1}{2}} e^{i\Theta_{k_1, \dots, k_N}} |k_1, \dots, k_N\rangle, \quad (4.16)$$

with

$$\Theta_{j_1, \dots, j_N} = \Theta_0 + \phi_{j_1} + \phi_{j_2} + \dots + \phi_{j_N}, \quad (4.17)$$

and Θ_0 a global phase.

In order to prove Thm. 4, we shall initially derive a suitable expression for the occupation number $\Lambda = \langle \psi_N | \hat{n}_{|\varphi\rangle} | \psi_N \rangle$ of single-particle orbitals in pure N -hardcore boson states (Sec. 4.3.1). By promoting this functional to an action and implementing normalisation constraints using Lagrange multipliers, we derive a set of Euler-Lagrange equations in Sec. 4.3.2. The equations are solved and the solutions are discussed and extended to mixed states, which completes the proof of Thm. 4. In Sec. 4.3.3, some properties of λ_{max} and $|\psi_N^{\lambda_{max}}\rangle$ shall be explored. Following that, a particular physically relevant basis of states unbiased to the hardcore basis, the Bloch-states, will be considered in detail and the structure of the corresponding states $|\psi_N^{\lambda_{max}}\rangle$ will be related to N -permanents of Bloch-states in Sec. 4.3.4.

4.3.1 Derivation of a functional Λ for hardcore boson single-particle state occupation numbers

In this section, we are going to derive a simplified form of the expression for the occupation number Λ of a single-particle state $|\varphi\rangle$ in an N -hardcore boson state $|\psi_N\rangle$:

$$\Lambda(|\varphi\rangle, |\psi_N\rangle) := \langle \psi_N | \hat{n}_{|\varphi\rangle} | \psi_N \rangle. \quad (4.18)$$

Any arbitrary single particle state $|\varphi\rangle$ can be expanded in terms of the hardcore basis $\mathcal{B}_{hcb}$:

$$|\varphi\rangle = \sum_{i=1}^d c_i |i\rangle. \quad (4.19)$$

Let $\hat{b}_i^\dagger$ and $\hat{b}_j$ denote the ladder operators that correspond to $\mathcal{B}_{hcb}$. The occupation number operator $\hat{n}_{|\varphi\rangle}$ thus becomes:

$$\hat{n}_{|\varphi\rangle} = \sum_{i,j=1}^d c_i c_j^* \hat{b}_i^\dagger \hat{b}_j. \quad (4.20)$$

Next, we shall consider a suitable form of some (arbitrary) hardcore boson state $|\psi_N\rangle$. Recall that every pure hardcore boson state may be written as a superposition of bosonic permanents $|i_1, \dots, i_N\rangle$ of elements of $\mathcal{B}_{hcb}$. Each such permanent can be derived by the action of the annihilation operators $\hat{b}_i$ on the state $|\xi\rangle = |1, \dots, d\rangle$ of $N = d$ hardcore bosons on d lattice sites. Consequently, any arbitrary N -hardcore boson state may be decomposed as:

$$|\psi_N\rangle = \sum_{j_1=1}^d \dots \sum_{j_n=1}^d A_{j_1, j_2, \dots, j_n} \hat{b}_{j_1} \hat{b}_{j_2} \dots \hat{b}_{j_n} |\xi\rangle, \quad (4.21)$$

where $n = d - N$ represents the number of holes (see discussion below). Note that the sums over j_k have not been restricted to $j_{k+1} > j_k$. Therefore, Eq. (4.21) comprises $n!$ copies of each permanent. The advantage of this choice will become clearer in the derivation of Λ below. Without loss of generality, one can choose the coefficients $A_{\dots}$ to be totally symmetric and in addition, set those coefficients in which at least two indices coincide to zero:

$$A_{j_1, \dots, j_n} = \frac{1}{n!} \sum_{\sigma \in S_n} A_{\sigma(j_1), \dots, \sigma(j_n)}, \quad A_{\dots, k, \dots, k, \dots} = 0. \quad (4.22)$$

Finally, observe that since the expansion (4.21) contains $n!$ copies of the same permanents, the normalisation condition on $|\psi_N\rangle$ translates into

$$\sum_{j_1=1}^d \dots \sum_{j_n=1}^d |A_{j_1, j_2, \dots, j_n}|^2 = \frac{1}{n!}. \quad (4.23)$$

We now simplify the form of the occupation number Λ (4.18). By substitution of (4.21) and (4.20) into (4.18) one yields:

$$\Lambda = \sum_{\mathbf{j}} \sum_{\mathbf{k}} \sum_{m, l} A_{j_1, \dots, j_n}^* A_{k_1, \dots, k_n} c_m c_l^* \langle \xi | \hat{b}_{j_1}^\dagger \dots \hat{b}_{j_n}^\dagger \hat{b}_m^\dagger \hat{b}_l \hat{b}_{k_1} \dots \hat{b}_{k_n} | \xi \rangle. \quad (4.24)$$

The matrix elements of the ladder operator products can only assume values of 0 or 1. This can be used to carry out the sums over $\mathbf{k}$ and l . In order not to vanish, the matrix elements $\langle \xi | \hat{b}_{j_1}^\dagger \dots \hat{b}_{j_n}^\dagger \hat{b}_m^\dagger \hat{b}_l \hat{b}_{k_1} \dots \hat{b}_{k_n} | \xi \rangle$ have to satisfy the following two conditions:

1. Both sets of indices, $\{\mathbf{j}, m\}$ and $\{\mathbf{k}, l\}$, have each to be pairwise distinct, i.e. $m \neq j_1, \dots, j_n$ and $j_g \neq j_h$, as well as $l \neq k_1, \dots, k_n$ and $k_g \neq k_h$.
2. $(\mathbf{k}, l)$ must be a permutation of $(\mathbf{j}, m)$.

The first condition allows us to drop all elements of the sums over m and l for which $m \in \mathbf{j}$ and $l \in \mathbf{k}$. Note that due to the appropriate choice of the $A_{\dots}$ coefficients (4.22) the pairwise distinctness of elements of $\mathbf{j}$ and $\mathbf{k}$ does not require the adjustment of the sums over $\mathbf{j}$ and $\mathbf{k}$.

$$\Lambda = \sum_{\mathbf{j}} \sum_{m|m \notin \mathbf{j}} \left(\sum_{\mathbf{k}} \sum_{l|l \notin \mathbf{k}} A_{j_1, \dots, j_n}^* A_{k_1, \dots, k_n} c_m c_l^* \langle \xi | \hat{b}_{j_1}^\dagger \dots \hat{b}_{j_n}^\dagger \hat{b}_m^\dagger \hat{b}_l \hat{b}_{k_1} \dots \hat{b}_{k_n} | \xi \rangle \right). \quad (4.25)$$

The second condition can be implemented by replacing the two inner sums with a sum over all permutations of $n+1$ elements. The resulting expression then only includes the non-vanishing matrix elements, which therefore can be omitted:

$$\Lambda = \sum_{\mathbf{j}} \sum_{m|m \notin \mathbf{j}} \left(\sum_{\sigma \in S_{n+1}} A_{j_1, \dots, j_n}^* c_m A_{\sigma(j_1), \dots, \sigma(j_n)} c_{\sigma(m)}^* \right). \quad (4.26)$$

In a next step, one can split the sum over all permutations into a sum over the set of those permutations for which $\sigma(m) = m$ and a sum over the respective complement:

$$\Lambda = \sum_{\mathbf{j}} \sum_{m|m \notin \mathbf{j}} \left(\sum_{\substack{\sigma \in S_{n+1} \\ \sigma(m)=m}} A_{j_1, \dots, j_n}^* c_m A_{\sigma(j_1), \dots, \sigma(j_n)} c_{\sigma(m)}^* + \sum_{\substack{\sigma \in S_{n+1} \\ \sigma(m) \neq m}} A_{j_1, \dots, j_n}^* c_m A_{\sigma(j_1), \dots, \sigma(j_n)} c_{\sigma(m)}^* \right). \quad (4.27)$$

The left inner sum contains $n!$ elements of the same value due to the total symmetry of A . The right inner sum may be evaluated by considering the n different choices for $\sigma(m)$, i.e. $\sigma(m) = j_1, \dots, j_n$, which, together with the symmetry of A , leads to a factor of n . The remaining possible permutations contribute an additional factor of $(n!)$:

$$\Lambda = \sum_{\mathbf{j}} \sum_{m|m \notin \mathbf{j}} \left(n! \cdot |A_{j_1, \dots, j_n}|^2 |c_m|^2 + n \cdot n! \cdot A_{j_1, \dots, j_n}^* c_m A_{m, j_2, \dots, j_n} c_{j_1}^* \right). \quad (4.28)$$

The constrained sum over m can be written as the difference of two sums:

$$\begin{aligned} \Lambda &= \sum_{\mathbf{j}} \sum_{m=1}^d \left(n! \cdot |A_{j_1, \dots, j_n}|^2 |c_m|^2 + n \cdot n! \cdot A_{j_1, \dots, j_n}^* c_m A_{m, j_2, \dots, j_n} c_{j_1}^* \right) \\ &\quad - \sum_{\mathbf{j}} \sum_{m \in \mathbf{j}} \left(n! \cdot |A_{j_1, \dots, j_n}|^2 |c_m|^2 + n \cdot n! \cdot A_{j_1, \dots, j_n}^* c_m A_{m, j_2, \dots, j_n} c_{j_1}^* \right). \end{aligned} \quad (4.29)$$

By carrying out the second sum over m , the first term in the lower brackets will pick up a factor of n due to the symmetry of A , whereas in the second term only $m = j_1$

will be non-zero.

$$\begin{aligned} \Lambda = & \sum_j \sum_{m=1}^d \left(n! \cdot |A_{j_1, \dots, j_n}|^2 |c_m|^2 + n \cdot n! \cdot A_{j_1, \dots, j_n}^* c_m A_{m, j_2, \dots, j_n} c_{j_1}^* \right) \\ & - \sum_j \left(n \cdot n! \cdot |A_{j_1, \dots, j_n}|^2 |c_{j_1}|^2 + n \cdot n! \cdot A_{j_1, \dots, j_n}^* c_{j_1} A_{j_1, j_2, \dots, j_n} c_{j_1}^* \right). \end{aligned} \quad (4.30)$$

By renaming indices and using the normalisation conditions on $|\varphi\rangle$ and $|\psi_N\rangle$ (4.23), one now obtains a compact expression for Λ :

$$\Lambda = 1 + n \cdot n! \sum_{j_2 \dots j_n} \left| \sum_m c_m A_{m, j_2, \dots, j_n} \right|^2 - 2n \cdot n! \sum_{j_2 \dots j_n} \left(\sum_m |c_m|^2 |A_{m, j_2, \dots, j_n}|^2 \right). \quad (4.31)$$

The simplified structure of Λ becomes more apparent by looking at the A coefficients as a set of vectors labelled by $(n-1)$ indices $j_2, \dots, j_n$ with vector index m . The second term in (4.31) comprises of a sum of scalar products of these vectors with the c -vector of the single-particle state. The third term is built up by products of absolute squared components from those vectors. This term is therefore independent of the phases of c and A . The only phase dependence of Λ is given by the second term in which only the relative phases of c and A enter. All phases of c can thus be absorbed into the A coefficients. More fundamentally, this corresponds to a unitary transformation $|j\rangle \mapsto e^{-i\phi_j} |j\rangle$ of the one-particle basis $\mathcal{B}_{hcb}$, where ϕ_j represents the phase of the j -th coefficient of c . The transformed basis also satisfies the hardcore constraint. For each possible value of Λ one can find a state such that the one-particle state $|\varphi\rangle$ is a real-valued expansion of the underlying hardcore basis.

4.3.2 Global maximum of the Λ -functional

In order to determine the maximal single-particle state occupation number of hardcore boson states, one has to consider the Euler-Lagrange equations related to the expression of the occupation number functional Λ (4.31). It will prove helpful to introduce the polar decompositions of the c and A coefficients,

$$c_m = r_m e^{i\phi_m} \quad \text{and} \quad A_{j_1, \dots, j_n} = a_{j_1, \dots, j_n} e^{i\theta_{j_1, \dots, j_n}}, \quad (4.32)$$

such that the action becomes:

$$\begin{aligned} S[r, \phi, a, \theta, \mu, \nu] = & n \cdot n! \sum_{j_2 \dots j_n} \left\{ \left| \sum_m r_m e^{i\phi_m} a_{m, j_2, \dots, j_n} e^{i\theta_{m, j_2, \dots, j_n}} \right|^2 - 2 \sum_m r_m^2 a_{m, j_2, \dots, j_n}^2 \right\} \\ & + 1 + \nu \left(\sum_m (r_m^2) - 1 \right) + \mu \left(\sum_{j_1 \dots j_n} (a_{j_1, \dots, j_n}^2) - \frac{1}{n!} \right). \end{aligned} \quad (4.33)$$

Note that Lagrange multipliers μ and ν have been introduced to enforce the normalisation of $|\varphi\rangle$ and $|\psi_N\rangle$ to unity, (4.23). The variation of the action S though, may still lead to negative values for r and a . This means that in a strict sense the non-negativity of these variables would have to be imposed on the system by using the KKT-formalism.⁴ Every solution involving negative r or a however, can be related to another solution with equal value of S and positive r or a through a shift of the respective phases by $\pm\pi$. We thus proceed without implementing further constraints of the KKT-formalism.

The Euler-Lagrange equations for ϕ_m and $\theta_{m,j_2,\dots,j_n}$ are derived as:

$$0 = r_m e^{i\phi_m} \sum_{j_2 \dots j_n} \left(a_{m,j_2,\dots,j_n} e^{i\theta_{m,j_2,\dots,j_n}} \sum_k r_k e^{-i\phi_k} a_{k,j_2,\dots,j_n} e^{-i\theta_{k,j_2,\dots,j_n}} \right) - h.c. , \quad (4.34a)$$

$$0 = r_m e^{i\phi_m} a_{m,j_2,\dots,j_n} e^{i\theta_{m,j_2,\dots,j_n}} \sum_k r_k e^{-i\phi_k} a_{k,j_2,\dots,j_n} e^{-i\theta_{k,j_2,\dots,j_n}} - h.c. \quad (4.34b)$$

By summing over the free indices j_2 to j_n , one immediately recognises that Eq. (4.34b) implies Eq. (4.34a). Observe that solutions of Eq. (4.34b) for which the sum over k vanishes correspond to $S[\cdot] = \Lambda < 1$ (4.33) and may therefore be disregarded. Consequently, for the phases whose corresponding amplitudes r_m are not zero, the solution to Eq. (4.34b) has to fulfil:

$$\phi_m + \theta_{m,j_2,\dots,j_n} = (const.)_{j_2 \dots j_n} \quad \forall m = 1 \dots d , \quad (4.35)$$

where the constants depend on the indices j_2 to j_n .

The Euler-Lagrange equations for the amplitudes $r_{\dots}$ and $a_{\dots}$ may be written in the following form:

$$0 = n n! \sum_{j_2 \dots j_n} \left\{ \left(e^{i(\phi_m + \theta_{m,j_2,\dots,j_n})} a_{m,j_2,\dots,j_n} \sum_k r_k a_{k,j_2,\dots,j_n} e^{-i(\theta_{k,j_2,\dots,j_n} + \phi_k)} \right) + h.c. \right\} \\ + 2 \nu r_m - 4n n! \sum_{j_2 \dots j_n} r_m (a_{m,j_2,\dots,j_n})^2, \quad (4.36a)$$

$$0 = n n! \left\{ \left(e^{i(\phi_m + \theta_{m,j_2,\dots,j_n})} \sum_k r_k a_{k,j_2,\dots,j_n} e^{-i(\phi_k + \theta_{k,j_2,\dots,j_n})} \right) + h.c. \right\} \cdot r_m \\ + 2 \mu a_{m,j_2,\dots,j_n} - 4n n! r_m^2 a_{m,j_2,\dots,j_n} . \quad (4.36b)$$

⁴Solutions of constrained optimisation problems may be determined by using the Karush-Kuhn-Tucker (KKT) formalism. An introduction to this technique, which will also be used in subsequent sections, is provided in the appendix, Sec. D

In order to determine the values of the Lagrange multipliers μ and ν one can multiply Eq. (4.36a) with r_m and Eq. (4.36b) with $a_{m,j_2,\dots,j_n}$, and sum over all free indices:

$$\nu = \frac{\mu}{n!} = -n \, n! \sum_{j_2 \dots j_n} \left(\left| \sum_m c_m A_{m,j_2,\dots,j_n} \right|^2 - 2 \sum_m (|c_m|^2 |A_{m,j_2,\dots,j_n}|^2) \right) \stackrel{!}{=} -S[\cdot] + 1. \quad (4.37)$$

Both values are directly related to the value of the functional. Recalling the original form of the functional as an expectation value of a positive operator (4.18) one can conclude that ν and μ must always be less than or equal to one. Since we are interested in finding the global maximum we can even restrict to solutions for which $\nu \leq 0$.⁵ In that case, Eq. (4.36b) implies that if $r_m = 0$, then also $a_{m,j_2,\dots,j_n} = 0$ for all choices of indices $j_2, \dots, j_n$. Due to Eq. (4.36a), a converse statement holds true for sums of $a_{m,j_2,\dots,j_n}$. If we consider solutions in which p different amplitudes r_m become zero, the Euler-Lagrange equations for a setting of N particles on d sites (4.34) and (4.36) will reduce to the respective equations for the setting of $N - p$ particles on $d - p$ sites. The result for the maximal occupation number derived further below will prove to be strictly monotonic increasing.⁶ We shall therefore *a priori* assume that $r_m > 0, \forall m = 1 \dots d$.

The Euler-Lagrange equations (4.36) can now be simplified by inserting the phase relations (4.35):

$$0 = \sum_{j_2 \dots j_n} \left(a_{m,j_2,\dots,j_n} \sum_k r_k a_{k,j_2,\dots,j_n} \right) + \frac{\nu}{n \, n!} r_m - 2 \sum_{j_2 \dots j_n} r_m (a_{m,j_2,\dots,j_n})^2, \quad (4.38a)$$

$$0 = r_m \sum_k r_k a_{k,j_2,\dots,j_n} + \frac{\mu}{n \, n!} a_{m,j_2,\dots,j_n} - 2 r_m^2 a_{m,j_2,\dots,j_n}. \quad (4.38b)$$

Since this is a set of multivariate quartic equations, determining all of their solutions will generally prove to be difficult. In order to circumvent this obstacle, one may regard the Euler-Lagrange equations (4.38) as dynamical equations of a simplified action S' :

$$S'[r, a, \mu', \nu'] = \sum_{j_2 \dots j_n} \left\{ \left| \sum_m r_m a_{m,j_2,\dots,j_n} \right|^2 - 2 \sum_m r_m^2 a_{m,j_2,\dots,j_n}^2 \right\} + \nu' \left(\sum_m (r_m^2) - 1 \right) + \mu' \left(\sum_{j_1 \dots j_n} (a_{j_1,\dots,j_n}^2) - \frac{1}{n!} \right). \quad (4.39)$$

⁵The global minimum is obviously given by $\Lambda_{min} = 0$. Solutions of the Euler-Lagrange equations which correspond to this value of the occupation number are, for example, given by one-particle states $|\phi\rangle$ which have zero overlap with those states building up the permanents of the N -hardcore boson state. Clearly, the global maximum will at least take the value 1.

⁶By strictly monotonic increasing it is meant that $\lambda_{max}(N+1, d+1) > \lambda_{max}(N, d)$.

By carefully applying the Cauchy-Schwarz inequality to the first term in the curly brackets, one obtains another action $\bar{S}$ whose extremal points will constitute upper limits to the maximal occupation number. Because of the symmetry properties of the $a_{\dots}$ coefficients (4.22) the first term is seen to be bounded by:

$$\begin{aligned} \left| \sum_m r_m a_{m,j_2,\dots,j_n} \right|^2 &\stackrel{(4.22)}{=} \left| \sum_{\substack{m: \\ m \neq j_2 \dots j_n}} r_m a_{m,j_2,\dots,j_n} \right|^2 \leq \left(\sum_{\substack{m: \\ m \neq j_2 \dots j_n}} r_m^2 \right) \left(\sum_{\substack{k: \\ k \neq j_2 \dots j_n}} (a_{k,j_2,\dots,j_n})^2 \right) \\ &\stackrel{(4.22)}{=} \left(\sum_m r_m^2 - \sum_{m=j_2 \dots j_n} r_m^2 \right) \sum_k (a_{k,j_2,\dots,j_n})^2. \end{aligned} \quad (4.40)$$

This implies that an upper bound to the functional S' (4.39) is given by:

$$\begin{aligned} \bar{S}[r, a, \mu', \nu'] &= \sum_{j_2 \dots j_n} \left\{ \left(\sum_m r_m^2 - \sum_{m=j_2 \dots j_n} r_m^2 \right) \sum_k (a_{k,j_2,\dots,j_n})^2 - 2 \sum_m r_m^2 a_{m,j_2,\dots,j_n}^2 \right\} \\ &\quad + \nu' \left(\sum_m (r_m^2) - 1 \right) + \mu' \left(\sum_{j_1 \dots j_n} (a_{j_1,\dots,j_n}^2) - \frac{1}{n!} \right) \geq S'. \end{aligned} \quad (4.41)$$

The Euler-Lagrange equations of this new functional are computed as:

$$0 = r_m \left[\frac{1}{n!} - (n+1) \sum_{j_2 \dots j_n} (a_{m,j_2,\dots,j_n})^2 + \nu \right], \quad \forall m = 1 \dots d; \quad (4.42a)$$

$$0 = a_{m,j_2,\dots,j_n} \left[1 - \sum_{k=j_2 \dots j_n} (r_k)^2 - 2(r_m)^2 \right], \quad \forall \{m, j_2, \dots, j_n\} \in \mathbb{P}_n^d. \quad (4.42b)$$

Note that the form of both equations has already been simplified by using the normalisation conditions. From the second equation (4.42b) we can deduce that r_m is constant for all $m = 1 \dots d$. Due to Eq. (4.42a), the same holds true for partial sums of $(a_{m,j_2,\dots,j_n})^2$. Using the proper normalisations we can therefore conclude that:

$$r_m = 1/\sqrt{d} \quad \text{and} \quad \sum_{j_2,\dots,j_n} (a_{m,j_2,\dots,j_n})^2 = 1/(n!d), \quad \forall m = 1 \dots d. \quad (4.43)$$

The manifold of points fulfilling the two equations (4.43) are potential extremal points of the action $\bar{S}$ since they solve the related Euler-Lagrange equations (4.42). In order to check whether these points represent local maxima, one can consider the Hessian of the functional (4.41) and examine its eigenvalues. This unfortunately proves to be a cumbersome task.⁷ We shall thus choose a more direct approach and check the

⁷Of course, since the functional $\bar{S}$ is a quadratic form, its Hessian is a constant matrix. Nevertheless, determining the signs of the eigenvalues is generally not feasible.

values of the action $\bar{S}$ at points of the solution manifold defined by (4.43):

$$\begin{aligned} \bar{S} \Big|_{\substack{r_m=1/\sqrt{d}; \\ \sum_{j_2 \dots j_n} (a_{m,j_2, \dots, j_n})^2 \\ = 1/(n!d)}} &= \sum_{j_2 \dots j_n} \left(\left(1 - \frac{n-1}{d}\right) \sum_m (a_{m,j_2, \dots, j_n})^2 - 2 \sum_m \frac{1}{d} (a_{m,j_2, \dots, j_n})^2 \right) \\ &= \frac{1}{n!} \left(1 - \frac{n+1}{d}\right). \end{aligned} \quad (4.44)$$

The functional assumes the same value at all points defined by (4.43). Hence, (4.44) indeed represents the global maximum of $\bar{S}$. If $\bar{S}$ were to assume a larger value on the boundary of the constrained parameter domain of r and a , at least one r_m would have to be zero according to the KKT-formalism. This scenario, however, has been discussed above and related to a setting with reduced particle number and number of sites (cf. remarks following Eq. (4.37)).

Let us now consider the relation between $\bar{S}$ and S' (4.41) again. For sets of fixed indices $j_2, \dots, j_n$ define the $(d-n+1)$ -dimensional vectors $\vec{a}_{j_2, \dots, j_n} = (a_{m,j_2, \dots, j_n})_{m \neq j_2 \dots j_n}$. On the basis of Cauchy-Schwarz, the equality of $\bar{S}$ with S' is achieved if and only if all vectors $\vec{a}_{j_2, \dots, j_n}$ are parallel to the vector with constant coefficients r_m . This set of coefficients is contained within the solution manifold (4.43). Because $\bar{S}$ constitutes an upper bound to S' , the global maximum of S' is also given by (4.44) and achieved for constant vectors (r_m) and $\vec{a}_{j_2, \dots, j_n}$. The scheme further translates to the original action S . Using the normalisation constraints, the functional S thus assumes its global maximum at:

$$r_m = 1/\sqrt{d}, \quad a_{j_1, \dots, j_n} = \frac{1}{n! \sqrt{\binom{d}{n}}}, \quad \phi_m + \theta_{m,j_2, \dots, j_n} = \text{const.}, \quad \forall m = 1 \dots d, \quad \mathbf{j} \in \mathbb{P}_n^d. \quad (4.45)$$

The value of S at these coefficients is given by:

$$\begin{aligned} \lambda_{max} = S \Big|_{(4.45)} &= 1 + n n! \sum_{j_2 \dots j_n} \left(\left| \sum_{m \neq j_2 \dots j_n} d^{-\frac{1}{2}} \frac{1}{n!} \binom{d}{n}^{-\frac{1}{2}} \right|^2 - 2 \sum_{l \neq j_2 \dots j_n} d^{-1} \frac{1}{(n!)^2} \binom{d}{n}^{-1} \right) \\ &= 1 + \left(n - \frac{n^2}{d} - \frac{n}{d} \right). \end{aligned} \quad (4.46)$$

Expressed in terms of the particle number $N = d-n$, the maximal occupation number reads as:

$$\lambda_{max}(N, d) = \frac{N}{d} (d - N + 1). \quad (4.47)$$

As mentioned before, this result increases strictly monotonically with the number of particles and sites in the sense that $\lambda_{max}(N+1, d+1) > \lambda_{max}(N, d)$ for $N < d$.

In the next step, we shall more closely examine the structure of the states and single particle orbitals for which λ_{max} is achieved.

The equal weight of all amplitudes r_m (4.45) confirms that $|\varphi\rangle$ is unbiased with respect to the hardcore basis. The phases ϕ_m however, are not uniquely determined in agreement with the comments made at the end of the previous section, Sec. 4.3.1. The amplitudes $a_{j_1, \dots, j_n}$ may be related to the form of $|\psi_N\rangle$ (4.16) by recalling that in their definition (4.21) they have been purposely overcounted. The total symmetry cancels the factor $n!$ and the binomial identity $\binom{d}{n} = \binom{d}{d-n} = \binom{d}{N}$ establishes the desired result (4.16).

The phases $\Theta_{i_1, \dots, i_N}$ of the expansion coefficients of $|\psi_N\rangle$ (4.17) can be uniquely determined up to a global phase factor. Given a fixed set of phases ϕ_m let us choose the global phase factor such that

$$\theta_{(d-n+1), \dots, d} = \phi_1 + \phi_2 + \dots + \phi_N. \quad (4.48)$$

By using Eq. (4.35) one can compute other phases, e.g.

$$\theta_{(d-n), (d-n+2), \dots, d} = \theta_{(d-n+1), \dots, d} - \phi_{(d-n)} + \phi_{(d-n+1)} = \phi_1 + \phi_2 + \dots + \phi_{N-1} + \phi_{N+1}. \quad (4.49)$$

The scheme may be extended to all phases: For any set $\{j_1, \dots, j_d\}$ which is a permutation of $\{1, \dots, d\}$ the phase $\theta_{j_1, \dots, j_n}$ is given by:

$$\theta_{j_1, \dots, j_n} = \phi_{j_{n+1}} + \phi_{j_{n+2}} + \dots + \phi_{j_d}. \quad (4.50)$$

Since in the expansion of $|\psi_N\rangle$ (4.21) the phase factor $e^{i\theta_{j_1, \dots, j_n}}$ belongs to the permanent $|j_{n+1}, \dots, j_d\rangle$, this verifies Eq. (4.17) and confirms Thm. 4 for pure states.

In order to include mixed states recall that the 1-RDO of every mixed hardcore boson state can be convexly expanded in terms of 1-RDOs of pure states (cf. Eq. (4.7)). By using Weyl's inequalities⁸ [106] one finds that the upper bound for occupation numbers is still given by λ_{max} and further recognises that $\lambda_1 = \lambda_{max}$ can only be achieved for the pure state $|\psi_N^{\lambda_{max}}\rangle$. This completes the proof of Thm. 4 also for mixed states.

If one extends the scope of maximal hardcore boson occupation numbers to systems with variable particles numbers, Thm. 4 leads to the following corollary:

⁸Let A, B be hermitian operators with non-increasingly ordered spectra $\vec{\lambda}$ and $\vec{\tau}$. For the spectrum $\vec{\sigma}$ of $C = A + B$ it holds that $\sigma_{(i+j-1)} \leq \lambda_i + \tau_j$ where equality is achieved if the natural orbitals coincide.

Corollary 2 (Maximal occupation on the Fock space)

For the hardcore boson Fock space $\mathcal{F}_{hcb}[\mathcal{H}_1^{(d)}]$ based on a d -dimensional one-particle Hilbert space, the maximal single-particle state occupation number is given by:

$$\tilde{\lambda}_{max} := \max_{\substack{|\phi\rangle \in \mathcal{H}_1^{(d)} \\ |\psi\rangle \in \mathcal{F}_{hcb}}} (\langle \psi | \hat{n}_{|\phi\rangle} | \psi \rangle) = \begin{cases} \frac{(1+d)^2}{4d}, & \text{if } d \text{ is odd;} \\ \frac{1}{2}(1 + \frac{d}{2}), & \text{if } d \text{ is even.} \end{cases} \quad (4.51)$$

Proof: Consider $\lambda_{max}(N, d)$ as a function of N and determine its maximum for both cases of odd and even numbers of sites. Using Weyl's inequalities from Ref. [106] yields the desired result.

4.3.3 Structural properties of λ_{max} and the occupation number maximising state $|\psi_N^{\lambda_{max}}\rangle$

At first let us take a look at two different thermodynamic limits of λ_{max} . Define the filling factor $\nu = \frac{N}{d}$. By increasing the number of sites d while keeping ν constant, the maximal occupation number normalised to N approaches a value smaller than one:

$$\lim_{\substack{d \rightarrow \infty \\ \nu = \text{const.}}} \left(\frac{\lambda_{max}}{N} \right) = 1 - \nu. \quad (4.52)$$

This captures the interesting result that for half-filling of a large number of lattice sites $d \gg 1$, the maximal occupation number approaches $\frac{N}{2}$.

Another limit is given by increasing the number of sites while keeping the particle number constant:

$$\lim_{\substack{d \rightarrow \infty \\ N = \text{const.}}} (\lambda_{max}) = N. \quad (4.53)$$

In that case, the influence of the hardcore interaction on the upper bound of the occupation numbers becomes weaker and the limit of λ_{max} resembles the bounds on common bosonic systems. The overlap of the corresponding states $|\psi_N^{\lambda_{max}}\rangle$ (4.16) with the bosonic permanent of N single-particles states $|\varphi\rangle$ converges to unity (see discussion below in Sec. 4.3.4).

We shall now investigate the structure of $|\psi_N^{\lambda_{max}}\rangle$ (4.16) in more detail. The one-particle reduced density operator associated with $\rho_N = |\psi_N^{\lambda_{max}}\rangle \langle \psi_N^{\lambda_{max}}|$ can straight-

State $ \psi\rangle$	$\langle \hat{n}_{ a}\rangle^2$	$(\Delta n_{ a})^2$	$\langle \hat{n}_{ a}\hat{n}_{ b}\rangle$	$\langle \delta \hat{n}_{ a}\delta \hat{n}_{ b}\rangle$
BMI/FMI $\prod_{j=1}^d (\hat{a}_j^{\dagger(b/f)})^{n_j} \rangle$	n_a^2	0	$n_a n_b$	0
BCo $e^{-N/2} \prod_{j=1}^d e^{\sqrt{\frac{N}{d}} \hat{b}_j^\dagger} \rangle$	$\frac{N}{d} \left(1 + \frac{N}{d}\right)$	$\frac{N}{d}$	$\frac{N^2}{d^2}$	0
BSF $\frac{1}{\sqrt{N!}} \left(\sum_{j=1}^d \frac{1}{\sqrt{d}} \hat{b}_j^\dagger \right)^N \rangle$	$\frac{N(d+N-1)}{d^2}$	$\frac{N}{d} \left(1 - \frac{1}{d}\right)$	$\frac{N(N-1)}{d^2}$	$-\frac{N}{d^2}$
$ \psi_N^{\lambda_{max}}\rangle$	$\frac{N}{d}$	$\frac{N}{d} \left(1 - \frac{N}{d}\right)$	$\frac{N(N-1)}{d(d-1)}$	$-\frac{N(d-N)}{d^2(d-1)}$

Table 4.1: On-site occupation number expectations and variances as well as number and number-fluctuation correlations (from left to right) of various many-body states: bosonic and fermionic Mott insulators (BMI and FMI), the bosonic coherent state (BCo), the bosonic superfluid state (BSF) and $|\psi_N^{\lambda_{max}}\rangle$. Respective thermodynamic limits are presented in Tab. 4.2.

forwardly be computed. In the underlying hardcore basis its components read as:

$$\begin{aligned}
\left(\rho_1^{\lambda_{max}} \right)_{ij} &= \begin{pmatrix} \frac{N}{d} & \frac{N(d-N)}{d(d-1)} e^{i(\phi_1-\phi_2)} & \dots \\ \frac{N(d-N)}{d(d-1)} e^{i(\phi_2-\phi_1)} & \frac{N}{d} & \frac{N(d-N)}{d(d-1)} e^{i(\phi_2-\phi_3)} \\ \vdots & \frac{N(d-N)}{d(d-1)} e^{i(\phi_3-\phi_2)} & \ddots \end{pmatrix}_{ij} \\
&= \left(\frac{N(d-N)}{d(d-1)} \right) \underbrace{e^{i(\phi_i-\phi_j)}}_{E_{ij}} + \left(\frac{N(N-1)}{d(d-1)} \right) \mathbb{1}_{ij}.
\end{aligned} \tag{4.54}$$

The maximally occupied single-particle state $|\varphi\rangle$ determines the phases ϕ_m . It is a natural orbital of $\rho_1^{\lambda_{max}}$ with the non-degenerate eigenvalue λ_{max} .⁹ The remaining part of the eigenspace is spanned by eigenvectors of the $(d-1)$ -fold degenerate eigenvalue

$$\lambda' = \lambda_2 = \dots = \lambda_d = \frac{N(N-1)}{d(d-1)}. \tag{4.55}$$

A set of orthogonal eigenvectors that span the eigenspace of λ' is given by:

$$|e_k\rangle = \frac{1}{\sqrt{k(k-1)}} \left(\sum_{j=1}^{k-1} (e^{i\phi_j} |j\rangle) - (k-1)e^{i\phi_k} |k\rangle \right), \quad \forall k = 2 \dots d. \tag{4.56}$$

If $|\varphi\rangle$ is chosen to be a Bloch state, the eigenspace of λ' (4.56) will be spanned by all the other Bloch states (see Sec. 4.3.4).

An important set of quantities to classify and compare $|\psi_N^{\lambda_{max}}\rangle$ with other many-body quantum states is provided by the expectation values of the on-site occupation

⁹This may be seen as an immediate consequence of the Schur-Horn Lemma in that the largest diagonal entry of a matrix is bounded from above by the largest eigenvalue. Hence, by maximising a diagonal entry, one gets an eigenvalue.

State $ \psi\rangle$	$\lim_{d \rightarrow \infty} \langle \hat{n}_{ a}^2 \rangle _\nu$	$\lim_{d \rightarrow \infty} (\Delta n_{ a})^2 _\nu$	$\langle \hat{n}_{ a} \hat{n}_{ b} \rangle$	$\langle \delta \hat{n}_{ a} \delta \hat{n}_{ b} \rangle$
BMI/FMI	n_a^2	0	$n_a n_b$	0
BCo	$\nu(1 + \nu)$	ν	ν^2	0
BSF	$\nu(1 + \nu)$	ν	ν^2	0
$ \psi_N^{\lambda_{max}}\rangle$	ν	$\nu(1 - \nu)$	ν^2	0

Table 4.2: Thermodynamic limits of the on-site occupation number expectations and variances as well as number and number-fluctuation correlations of various many-body states (cf. Tab. 4.1). Limit values are displayed for the limit of increasing d while keeping the filling factor $\nu = \frac{N}{d}$ constant. The limits of all quantities under constant N approach zero.

number operators $\hat{n}_{|a} = \hat{b}_{|a}^\dagger \hat{b}_{|a}$, their fluctuations and correlations. Clearly, the occupation number expectation and its higher momenta at any site $a \in 1 \dots d$ are given by:

$$\langle \psi_N^{\lambda_{max}} | \hat{n}_{|a} | \psi_N^{\lambda_{max}} \rangle = \frac{N}{d}, \quad \text{and} \quad \langle \psi_N^{\lambda_{max}} | (\hat{n}_{|a})^p | \psi_N^{\lambda_{max}} \rangle = \frac{N}{d}, \quad \forall p = 2, 3, \dots \quad (4.57)$$

As a consequence, the variance of $\hat{n}_{|a}$ does not vanish for filling factors smaller than one:

$$(\Delta n_{|a})^2 = \frac{N}{d} \left(1 - \frac{N}{d} \right) = \nu(1 - \nu). \quad (4.58)$$

When looking at non-local pair correlations of the occupation numbers one finds that for any pair of sites $a \neq b$:

$$\langle \psi_N^{\lambda_{max}} | \hat{n}_{|a} \hat{n}_{|b} | \psi_N^{\lambda_{max}} \rangle = \frac{N(N-1)}{d(d-1)}. \quad (4.59)$$

In order to describe fluctuations, it is advantageous to introduce the fluctuation operator $\delta \hat{n}_{|a} = \hat{n}_{|a} - \langle \hat{n}_{|a} \rangle$. The expectation value of its square defines the variance (4.58). Furthermore, it can be used to determine the non-local number-fluctuation correlations which assume the same value for any arbitrary pair of sites $a \neq b$:

$$\langle \psi_N^{\lambda_{max}} | \delta \hat{n}_{|a} \delta \hat{n}_{|b} | \psi_N^{\lambda_{max}} \rangle = -\frac{N(d-N)}{d^2(d-1)}. \quad (4.60)$$

A comparison of these characteristic values of $|\psi_N^{\lambda_{max}}\rangle$ with their counterparts from other states is shown in Tab. 4.1. For an introduction to various many-body quantum states see Refs. [58, 59].

The fermionic and bosonic Mott insulator states (FMI and BMI) can be written as single Slater determinants or bosonic permanents of the spatial basis, respectively. Both do not exhibit any fluctuations and are thus completely localised states. The bosonic coherent state (BCo) is a state with fluctuating total particle number.¹⁰ Despite this caveat, it shares some similarities with the $|\psi_N^{\lambda_{max}}\rangle$ state. For small filling factors $\nu = \frac{N}{d}$ the variances of the occupation numbers $(\Delta n_{|a\rangle})^2$ and their pair correlations $\langle \hat{n}_{|a\rangle} \hat{n}_{|b\rangle} \rangle$ approach the respective values of $|\psi_N^{\lambda_{max}}\rangle$. In contrast to $|\psi_N^{\lambda_{max}}\rangle$, however, the bosonic coherent state does not have any number-fluctuation correlations. A state which shares similar properties is given by the bosonic superfluid state. This state has negative number-fluctuation correlations, which for $d \gg N$ resemble those of the $|\psi_N^{\lambda_{max}}\rangle$ state:

$$\lim_{d \rightarrow \infty} \left(\frac{\langle \psi_{BSF} | \delta \hat{n}_{|a\rangle} \delta \hat{n}_{|b\rangle} | \psi_{BSF} \rangle}{\langle \psi_N^{\lambda_{max}} | \delta \hat{n}_{|a\rangle} \delta \hat{n}_{|b\rangle} | \psi_N^{\lambda_{max}} \rangle} \right) \Big|_N = 1. \quad (4.61)$$

Yet the number-fluctuation correlations of the $|\psi_N^{\lambda_{max}}\rangle$ and the superfluid state both separately approach zero under the thermodynamic limits.

In general, it is instructive to consider the two different thermodynamic limits of all these quantities for increasing d while keeping $\nu = \frac{N}{d}$ or just N constant (cf. Tab. 4.2). The limits emphasise that the bosonic superfluid state bears many similarities with the $|\psi_N^{\lambda_{max}}\rangle$ state. In particular, when $|\varphi\rangle$ is chosen to be the lowest Bloch state the corresponding state $|\psi_N^{\lambda_{max}}\rangle$ can be shown to be a projection of the bosonic superfluid state (cf. Sec. 4.3.4). Before doing so, we shall add a brief remark on the different characters of holes and particles in systems of hardcore bosons.

Already in Sec. 4.2 it has become apparent that the set of N -representable one-particle density operators is generally not isomorphic to the respective set for systems of $(d - N)$ hardcore bosons on d sites. The result on the maximal occupation number λ_{max} allows one to even strengthen this statement: If, in the spirit of the fermionic particle-hole transformation (cf. Eq. (2.32)), one were to define a transformation $(\hat{b}_i, \hat{b}_j^\dagger)_{particle} \mapsto (\hat{b}_i^\dagger, \hat{b}_j)_{hole}$, the occupation number expectations of the holes could achieve negative values since $\lambda_{max} > 1$ for $1 < N < d$. This inconsistency originates in the form of the on-site interaction term $U \sum_i (\hat{n}_i (\hat{n}_i - 1))$ which defines the hardcore boson space. Under the naively proposed particle hole transformation it will change to $U \sum_i (\hat{n}_i (\hat{n}_i + 1))$, which does not give rise to the hardcore boson space of $n = d - N$

¹⁰The total particle number operator $\hat{N} = \sum_i \hat{b}_{|i\rangle}^\dagger \hat{b}_{|i\rangle}$ does not fluctuate for the Mott insulator, superfluid and $|\psi_N^{\lambda_{max}}\rangle$ states, i.e. $(\Delta N)^2 = 0$. For the bosonic coherent state, however, one gets $(\Delta N)^2 = N$.

particles on d sites. By physical intuition, one may say that in contrast to the particles, the holes in systems of hardcore bosons do not exert a repulsive force on one another. If existent, a concept of particle-hole similarity for hardcore bosons will be more intricate than for fermions.

4.3.4 Maximal occupation and momentum eigenstates

Having studied the properties of $|\psi_N^{\lambda_{max}}\rangle$ for arbitrary defining orbitals $|\varphi\rangle$, unbiased to the hardcore basis $\mathcal{B}_{hcb} \equiv \{|i\rangle_x\}_{i=1}^d$ (recall Thm. 4), we shall now focus on states of particular physical relevance: the Bloch states $|k\rangle_p$ associated with $\mathcal{B}_{hcb}$.

$$|\varphi_k\rangle = |k\rangle_p := \frac{1}{\sqrt{d}} \sum_{j=1}^d e^{+2\pi i j k/d} |j\rangle_x, \quad \forall k = 1 \dots d. \quad (4.62)$$

As a consequence, the phases of the expansion coefficients of $|\psi_N^{\lambda_{max}}\rangle$ (4.16) and the matrix elements E_{ij} in the representation of ρ_1 (4.54) simplify significantly:

$$\Theta_{j_1, \dots, j_N} = \frac{2\pi}{d} k(j_1 + \dots + j_N), \quad E_{ij} = e^{\frac{2\pi}{d} k(i-j)}. \quad (4.63)$$

The eigenspace of the corresponding one-particle density operator is spanned by $|k\rangle_p$ with eigenvalue λ_{max} and the remaining Bloch states $\{|k'\rangle_p\}_{k' \neq k}$ with the $(d-1)$ -fold degenerate eigenvalue λ' (4.55). This can either be proven by direct computation or may be concluded from the translational invariance of $|\psi_N^{\lambda_{max}}\rangle$.¹¹

In order to gain further structural insight into the state $|\psi_N^{\lambda_{max}}\rangle$, one may look at its expansion in terms of bosonic permanents of Bloch states. The one-particle Fourier transformation (4.62) induces a unitary transformation on the N -particle Hilbert spaces of fermions and bosons. One generally finds that the fermionic Slater determinants $|k_1, k_2, \dots, k_N\rangle_p^{(f)}$ and bosonic permanents $|k_1, k_2, \dots, k_N\rangle_p^{(b)}$ of N Bloch states $\{|k_i\rangle_p\}_{i=1}^N$ can be expressed via:

$$|k_1, k_2, \dots, k_N\rangle_p^{(f,b)} = \mathcal{N} \sum_{n_1=1}^d \dots \sum_{n_N=1}^d \left[e^{+\frac{2\pi i}{d}(n_1 k_1 + \dots + n_N k_N)} |n_1, n_2, \dots, n_N\rangle_x^{(f,b)} \right]. \quad (4.64)$$

Note that the normalisation constant $\mathcal{N}$ merely depends on the multiplicities of the k_i . For the sake of completeness of this thesis, a thorough derivation is presented in the appendix, Sec. C.

¹¹Let $\hat{T}_l$ denote the translation operator on $\mathcal{H}_1^{(d)}$. Since $\hat{T}_l^{\otimes N}$ constitutes a symmetry operation on $|\psi_N^{\lambda_{max}}\rangle$, i.e. $\hat{T}_l^{\otimes N} |\psi_N^{\lambda_{max}}\rangle = e^{i\Phi_l} |\psi_N^{\lambda_{max}}\rangle$, the one-particle reduced density operator $\rho_1^{\lambda_{max}}$ commutes with $\hat{T}_l$: $[\rho_1^{\lambda_{max}}, \hat{T}_l] = 0$. Both operators thus have a common eigensystem which is given by the Bloch states.

For fermions, the form of Eq. (4.64) may be processed further by omitting those terms in the sums over n_i which have a vanishing Slater determinant, i.e. terms with coinciding pairs of indices. Self-evidently, one may only choose a set of distinct k_i , which then yields:

$$|k_1, k_2, \dots, k_N\rangle_p^{(f)} = \mathcal{N} \sum_{\mathbf{n} \in \mathbb{P}_d^N} \left[\left(\sum_{\sigma(\mathbf{n}) \in S_N} e^{+\frac{2\pi i}{d} \mathbf{k} \cdot \sigma(\mathbf{n})} (-1)^{\text{sign}[\sigma]} \right) |n_1, n_2, \dots, n_N\rangle_x^{(f)} \right]. \quad (4.65)$$

The outer sum accounts for all N -subsets $\mathbf{n}$ of $\{1, \dots, d\}$ whereas the inner sum represents all terms resulting from permutations σ of a fixed $\mathbf{n}$.¹² As one might expect, a single fermionic Slater determinant of Bloch states is unbiased with respect to all Slater determinants of the hardcore basis states. It is thus the fermionic analogue of the $|\psi_N^{\lambda_{max}}\rangle$ state, (4.16). The results on occupation number variances, correlations and fluctuations of the hardcore boson state $|\psi_N^{\lambda_{max}}\rangle$, Eq. (4.57) to Eq. (4.60), are easily seen to translate to the fermionic states $|k_1, k_2, \dots, k_N\rangle_p$. All this raises the question whether $|\psi_N^{\lambda_{max}}\rangle$ can be more elegantly expressed in momentum space.

At a first glance, the bosonic version of Eq. (4.64) reveals that any expansion of a single permanent of Bloch-states involves spatial permanents which contain more than one boson per site and hence violate the hardcore constraint. It would therefore be desirable to only select the hardcore permanents from the expansion (4.64). This is facilitated by the hardcore space projector $\hat{K}$, Eq. (4.8).

Let us apply $\hat{K}$ to a bosonic permanent of Bloch states (4.64). As in the case of fermions, only permanents with single occupancies will enter the $\hat{K}$ -projected expansion on the right hand side. Hence, similar to Eq. (4.65), the sums over n_i can be rewritten bearing in mind the bosonic statistics:¹³

$$\hat{K} |k_1, k_2, \dots, k_N\rangle_p^{(b)} = \mathcal{N} \sum_{\mathbf{n} \in \mathbb{P}_d^N} \left[\left(\sum_{\sigma(\mathbf{n}) \in S_N} e^{+\frac{2\pi i}{d} \mathbf{k} \cdot \sigma(\mathbf{n})} \right) |n_1, n_2, \dots, n_N\rangle_x^{(b)} \right]. \quad (4.66)$$

If one further chooses all k_i to be equal, the inner sum results in an additional factor of $N!$ which can be absorbed into the normalisation constant. A comparison with the phases in Eq. (4.63) establishes the important result:

$$\hat{K} |k, k, \dots, k\rangle_p^{(b)} \propto |\psi_N^{\lambda_{max}}\rangle. \quad (4.67)$$

The state $|\psi_N^{\lambda_{max}}\rangle$ associated with a maximally occupied Bloch state $|k\rangle_p$ is given by a normalised projection of the bosonic permanent of N Bloch states $\hat{K} |k, k, \dots, k\rangle_p^{(b)}$.

¹²A list of examples may be found in the appendix, Tab. C.1 and Tab. C.2.

¹³Examples of projected momentum-space hardcore bosons states may be found in the appendix, tables C.3-C.7.

Moreover this also shows that the state $|\psi_N^{\lambda_{max}}\rangle$ for $d = k$ represents the projection of the general bosonic superfluid state $|\psi_{BSF}\rangle$ (cf. Sec. 4.3.3) onto the hardcore boson space. For $|\psi_{BSF}\rangle$, the expectation value of the momentum occupation number and its variance simply become:

$$\langle \psi_{BSF} | \hat{n}_{|d\rangle_p} | \psi_{BSF} \rangle = N, \quad \text{and} \quad (\Delta n_{|d\rangle_p})^2 = 0. \quad (4.68)$$

Their counterparts for $|\psi_N^{\lambda_{max}}\rangle$ read as λ_{max} and

$$(\Delta \hat{n}_{|d\rangle_p})^2 = \frac{2N}{d^2} (d + N - 1)(N - 1), \quad (4.69)$$

which *per definitionem* represents the variance of λ_{max} . Note that in the thermodynamic limit of increasing number of sites d and constant particle number N the variance of λ_{max} vanishes, i.e. $\lim_{d \rightarrow \infty} (\Delta \hat{n}_{|d\rangle_p})^2|_N = 0$. This again strongly suggests that by increasing the number of sites the hardcore constraint is weakened so that $|\psi_N^{\lambda_{max}}\rangle$ approaches the form of a superfluid state.

4.4 Conditions for one-body N -representability of hardcore boson states

The maximal possible occupation number λ_{max} derived in the previous section constitutes a constraint on the set of N -representable one-particle spectra. In the present section, we shall extend our investigation to the structure of hardcore boson states and determine conditions for their one-body N -representability.

In a first step, one has to consider what kind of information about the one-particle density operator will be required to describe the one-body N -representability. In Sec. 2.3, it was outlined that fermionic one-body N -representability can entirely be described in terms of the $\vec{\lambda}$ -vector. For any one-particle unitary transformation U_1 and one-particle density operator $\rho_1^{(f)}$ having an N -particle representation $\rho_N^{(f)}$, also $\tilde{\rho}_1^{(f)} = U_1 \rho_1^{(f)} U_1^\dagger$ is N -representable by $\tilde{\rho}_N^{(f)} = U_1^{\otimes N} \rho_N^{(f)} (U_1^\dagger)^{\otimes N}$. This especially implies that for some $\vec{\lambda}$ -vector which suffices the N -representability conditions, the attributed natural orbitals may be chosen arbitrarily as long as they form an orthonormal system.

By contrast, this deduction is not possible for hardcore bosons. For some arbitrary one-particle unitary transformation U_1 , the induced N -particle unitary transformation $U_N = U_1^{\otimes N}$ will generally not commute with the hardcore boson space projector $\hat{K}$ (see Eq. (4.8)). This imposes restrictions on the unitary equivalence of one-particle density operators. The one-particle density operator

$$\tilde{\rho}_1 = U_1 \rho_1^{(hcb)} U_1^\dagger \quad (4.70)$$

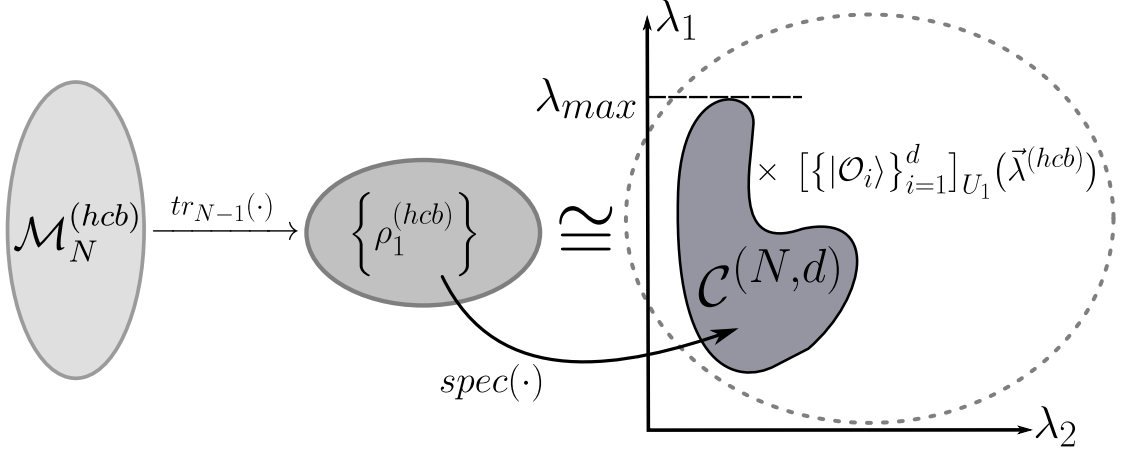


Figure 4.3: Sketch of the set $\mathcal{C}^{(N,d)}$ of compatible hardcore boson $\vec{\lambda}$ -vectors. The set of all N -representable one-particle density operators $\{\rho_1^{(hcb)}\}$ has a one-to-one correspondence to the product set of $\mathcal{C}^{(N,d)}$ and the pointwise defined classes of natural orbitals $[\{|\mathcal{O}_i\rangle\}_{i=1}^d]_{U_1}(\vec{\lambda}^{(hcb)})$. Note that the hyperplane defined by $\lambda_1 = \lambda_{max}$ touches $\mathcal{C}^{(N,d)}$ in exactly one point. For more details see text.

is only N -representable by

$$\tilde{\rho}_N = U_1^{\otimes N} \rho_N^{(hcb)} (U_1^\dagger)^{\otimes N}, \quad \text{if} \quad [U_1^{\otimes N}, \hat{K}] = 0. \quad (4.71)$$

A good example of this fact is given by the $|\psi_N^{\lambda_{max}}\rangle$ state and its associated one-particle density operator, Eq. (4.54). If one applies a unitary transformation to $\rho_1^{\lambda_{max}}$ which exchanges its natural orbitals $\{|\phi\rangle, |\mathbf{e}_i\rangle\}$ with the hardcore basis $\{|j\rangle\}_{j=1}^d$, then the resulting one-particle density operator violates the hardcore constraint.

In order to solve the N -representability problem for hardcore bosons, it is thus generally required to incorporate spectra *and* natural orbitals into the description. A form of restricted unitary equivalence (4.70) of hardcore boson one-particle density operators with identical spectrum is provided by the set of one-particle unitary transformations U_1 for which the induced N -particle transformation $U_1^{\otimes N}$ commutes with the projector $\hat{K}$. Therefore, to each compatible $\vec{\lambda}$ -vector one may associate an equivalence class of natural orbitals $[\{|\mathcal{O}_i\rangle\}_{i=1}^d]_{U_1}(\vec{\lambda}^{(hcb)})$.

In this section we are going to examine the set $\mathcal{C}^{(N,d)}$ of all $\vec{\lambda}$ -vectors which are *in principle* N -representable by a pure hardcore boson state of N particles on d sites. *In principle* here means that a compatible equivalence class of natural orbitals exists:

$$\mathcal{C}^{(N,d)} := \{spec(\rho_1) \mid \rho_1 = tr_{N-1}(|\psi_N^{(hcb)}\rangle \langle \psi_N^{(hcb)}|), |\psi_N^{(hcb)}\rangle \in \mathcal{H}_N^{(hcb)}\}. \quad (4.72)$$

An illustration of the set $\mathcal{C}^{(N,d)}$ may be found in Fig. 4.3.

How can one describe $\mathcal{C}^{(N,d)}$? The eigenvalues of a finite dimensional hermitian operator are completely determined by its characteristic polynomial, which in turn is uniquely defined by its coefficients. With the aid of the Faddeev and LeVerrier algorithm [42] all coefficients can be expressed in terms of the traces of the first d powers of ρ_1 :

$$0 = \det(\rho_1 - \lambda I) = \sum_{i=0}^d c_i \lambda^i; \quad c_{d-k} = -\frac{1}{k} \sum_{m=1}^k c_{d-k+m} \text{tr}(\rho_1^m) \quad (4.73)$$

This implies that for any d -tuple

$$t_d(\rho_1) := \{\text{tr}(\rho_1), \text{tr}(\rho_1^2), \dots, \text{tr}(\rho_1^d)\}, \quad (4.74)$$

the $\vec{\lambda}$ -vector associated with ρ_1 is uniquely determined by the following d equations:

$$\sum_{i=1}^d (\lambda_i)^k = \text{tr}(\rho_1^k), \quad \forall k = 1, \dots, d. \quad (4.75)$$

Therefore, a description of $\mathcal{C}^{(N,d)}$ shall be derived by specifying the set of all possible t_d tuples. In a first step, unrelated extremal values of $\text{tr}(\rho_1^k)$ are computed, which yields necessary conditions for the N -representability of $\vec{\lambda}$ -vectors.

4.4.1 Necessary conditions for N -representability

Let us begin by looking at systems with $(d-1)$ particles, i.e. systems with one hole. Since there can be no confusion with ρ_N we shall drop the index on ρ_1 in the remainder of this section.

4.4.1.1 Systems with $N = d-1$ particles

By using the annihilation operators $\hat{b}_i \equiv \hat{b}_{|i\rangle}$ and the d -particle state $|\xi\rangle$ (cf. Eq. (4.21)), any arbitrary pure state of $N = d-1$ particles can be decomposed as:

$$|\psi_{N=d-1}\rangle = \sum_{i=1}^d A_i \hat{b}_i |\xi\rangle. \quad (4.76)$$

Normalisation of $|\psi_{N=d-1}\rangle$ to unity imposes the standard condition $\sigma^{(2)} = 1$ onto the complex coefficients A_i , where for later use we have defined the sums of powers:

$$\sigma^{(i)} := \sum_{k=1}^d |A_k|^i. \quad (4.77)$$

The one-particle density operator of the state $|\psi_{N=d-1}\rangle$ assumes a simple form:

$$(\rho)_{ij} = (1 - 2|A_i|^2)\delta_{ij} + A_i A_j^* \quad (4.78)$$

The first four entries of the d -tuple t_d (4.74) may easily be computed and can solely be written in terms of the even power sums $\sigma^{(2n)}$:

$$\begin{aligned} \text{tr}(\rho) &= 2\sigma^{(2)}; \\ \text{tr}(\rho^2) &= d - 2\sigma^{(2)} + (\sigma^{(2)})^2; \\ \text{tr}(\rho^3) &= d - 3\sigma^{(2)} - 6\sigma^{(2)}\sigma^{(4)} + 4\sigma^{(6)} + 3(\sigma^{(2)})^2 + (\sigma^{(2)})^3; \\ \text{tr}(\rho^4) &= d - 4\sigma^{(2)} + 16\sigma^{(6)} - 16\sigma^{(8)} + 6(\sigma^{(2)})^2 + 4(\sigma^{(2)})^3 \\ &\quad - 24\sigma^{(2)}\sigma^{(4)} - 8(\sigma^{(2)})^2\sigma^{(4)} + 16\sigma^{(2)}\sigma^{(6)} + (\sigma^{(2)})^4 + 8(\sigma^{(4)})^2. \end{aligned} \quad (4.79)$$

Traces of higher powers of ρ will also depend solely on the even power sums $\sigma^{(2n)}$. The expressions of $\text{tr}(\rho^k)$ may be regarded as functionals of the coefficients A_i and one can derive the Euler-Lagrange equations of the corresponding action. Note that this requires one *not* to substitute the terms $\sigma^{(2)}$ by the normalisation 1 before carrying out the variation but rather to implement the constraint using a Lagrange multiplier.

A closer look at ρ^2 , however, already reveals an interesting property of all one-hole hardcore boson systems. Since $\rho^2 = d - 1$ is constant, no variation is required and one obtains:

$$(\lambda_1)^2 + (\lambda_2)^2 + \dots + (\lambda_d)^2 = d - 1. \quad (4.80)$$

Let us now more specifically consider the case of $d = 4$ lattice sites. In addition to the equality constraints given by the normalisation of ρ and the identity (4.80), one can determine the extremal values of $\text{tr}(\rho^3)$ by variation of the action:

$$S_3[A_i, \mu_1] := \text{tr}(\rho^3) - \mu_1(\sigma^{(2)} - 1). \quad (4.81)$$

The resulting Euler-Lagrange equations become a system of multivariate polynomial equations. By using an implementation of the Buchberger algorithm (cf. Ref. [14]) in the CAS Mathematica one gets a solution set (up to permutations and arbitrary phases) with a finite number of extremal values:

$$\begin{aligned} A_1 &= 0, A_2 = 0, A_3 = \sqrt{1 - (A_4)^2}, \mu_1 = 0, S_3 = 3; \\ A_1 &= \frac{1}{\sqrt{3}}, A_2 = \frac{1}{\sqrt{3}}, A_3 = \frac{1}{\sqrt{3}}, A_4 = 0, \mu_1 = -\frac{4}{3}, S_3 = \frac{31}{9}; \\ A_1 &= \frac{1}{2}, A_2 = \frac{1}{2}, A_3 = \frac{1}{2}, A_4 = \frac{1}{2}, \mu_1 = -\frac{9}{4}, S_3 = \frac{15}{4}; \end{aligned} \quad (4.82)$$

Without need for further analysis one can read off the maximum and minimum of $tr(\rho^3)$ to be $15/4$ and 3 , respectively.

Similarly, the extremal values of $tr(\rho^4)$ are found by solving the Euler-Lagrange equations of the action:

$$S_4[A_i, \mu_1] := tr(\rho^4) - \mu_1(\sigma^{(2)} - 1), \quad (4.83)$$

which yields:

$$\begin{aligned} A_1 = 0, A_2 = 0, A_3 = \sqrt{1 - (A_4)^2}, \mu_1 = 0, S_3 = 3; \\ A_1 = \frac{1}{\sqrt{3}}, A_2 = \frac{1}{\sqrt{3}}, A_3 = \frac{1}{\sqrt{3}}, A_4 = 0, \mu_1 = -\frac{80}{27}, S_3 = \frac{113}{27}; \\ A_1 = \frac{1}{2}, A_2 = \frac{1}{2}, A_3 = \frac{1}{2}, A_4 = \frac{1}{2}, \mu_1 = -6, S_3 = \frac{21}{4}. \end{aligned} \quad (4.84)$$

Together with the upper bound on the maximal occupation number, this forms our first result on necessary constraints for N -representability:

$$\begin{aligned} \lambda_1 + \lambda_2 + \lambda_3 + \lambda_4 = 3; \quad (\lambda_1)^2 + (\lambda_2)^2 + (\lambda_3)^2 + (\lambda_4)^2 = 3; \\ 3 \leq (\lambda_1)^3 + (\lambda_2)^3 + (\lambda_3)^3 + (\lambda_4)^3 \leq \frac{15}{4}; \\ 3 \leq (\lambda_1)^4 + (\lambda_2)^4 + (\lambda_3)^4 + (\lambda_4)^4 \leq \frac{21}{4}; \\ \lambda_1 \leq \lambda_{max}, \quad \lambda_{i+1} \leq \lambda_i. \end{aligned} \quad (4.85)$$

Note that these inequalities are not yet sufficient to guarantee N -representability. The reason for this is that we have not taken into account the boundary condition that is imposed upon the variation of S_4 by $tr(\rho^3)$ assuming a predetermined value in the range of $[3, 15/4]$. This will be done subsequently (cf. Sec. 4.4.2) by using another Lagrange multiplier μ_2 and including the term $\mu_2(tr(\rho^3) - \chi)$ to modify the action S_4 . Further notice that additional enforcement of the boundary condition $tr(\rho^2) = 3$ in the actions S_3 and S_4 is redundant as it leads to the same Euler-Lagrange equations.

In the structure of the solutions Eqs. (4.82) and Eqs. (4.84) one recognises the minimum to be achieved for a single bosonic permanent and the maximum to correspond to the previously described $|\psi_N^{\lambda_{max}}\rangle$ state. The restricting character of the conditions (4.85) becomes more obvious by comparing them with their analogues of common bosons:

$$\begin{aligned} \lambda_1 + \lambda_2 + \lambda_3 + \lambda_4 = 3; \\ \frac{9}{4} \leq (\lambda_1)^2 + (\lambda_2)^2 + (\lambda_3)^2 + (\lambda_4)^2 \leq 9; \\ \frac{27}{16} \leq (\lambda_1)^3 + (\lambda_2)^3 + (\lambda_3)^3 + (\lambda_4)^3 \leq 27; \\ \frac{81}{64} \leq (\lambda_1)^4 + (\lambda_2)^4 + (\lambda_3)^4 + (\lambda_4)^4 \leq 81. \end{aligned} \quad (4.86)$$

The second equality constraint is weakened and splits into two inequalities, whereas the upper and lower boundaries of $tr(\rho^3)$ and $tr(\rho^4)$ are extended.

The above derivation scheme can be generalised to arbitrary one-hole systems. Because one encounters similar structures of the states for which $tr(\rho^n)$ becomes extremal, the question arises whether the aforementioned form of necessary conditions might also be valid for arbitrary settings.

4.4.1.2 Arbitrary systems with N particles on d sites

In this paragraph, a general form of necessary conditions for N -representability shall be worked out by using the tools of constrained optimisation, which are also known as the Karush-Kuhn-Tucker formalism. For the sake of completeness of this thesis, an introduction to this lesser-known technique is provided in the appendix, Sec. D. The conditions will give rise to sets which are outer approximations of $\mathcal{C}^{(N,d)}$.

For N particles on a finite number of sites d , the trace of ρ^m can be expressed in terms of the $\vec{\lambda}$ -vector via Eq. (4.75). Formally, the extremal values of $tr(\rho^m)$ - when regarded as a functional - are yielded by variation over all $\vec{\lambda} \in \mathcal{C}^{(N,d)}$. This set, of course, is yet unknown. We shall therefore increase the domain of variation to all $\vec{\lambda}$ -vectors within the ' λ_{max} -cube', $\vec{\lambda} \in [0, \lambda_{max}^{(N,d)}]^d \supset \mathcal{C}^{(N,d)}$. A sketch of this concept is displayed in Fig. 4.4.

The extension of the variation domain makes it necessary to consider some aspects in more detail.

Firstly, if the global maximum of $tr(\rho^m)$ within the λ_{max} -cube is attained at a point $P_{max} \in \mathcal{C}^{(N,d)}$, then the oriented hyperplane

$$l_{max} := \left\{ \vec{\lambda} \mid \sum_i (\lambda_i)^m = tr(\rho^m) \Big|_{P_{max}} \right\} \quad (4.87)$$

provides an optimal bound. This means that no smaller value of $tr(\rho^m)$ may be used in the definition of l_{max} without l_{max} intersecting the set $\mathcal{C}^{(N,d)}$. The same holds for the global minimum. Both cases are schematically drawn in Fig. 4.4 (a). The λ_{max} -cube is indicated by the partially dotted black framed square. The dark grey set within the cube represents the set of ordered and normalised spectra $\mathcal{C}^{(N,d)}$. The points P_{max} and P_{min} (blue reticles) mark positions of the global maximum and minimum of $tr(\rho^m)$ achieved under the condition of a proper normalisation of $tr(\rho)$ to N . The red curved solid lines represent l_{max} and l_{min} .

Because $tr(\rho^m)$ is symmetric under arbitrary permutations of the λ_i , several equivalent solutions to the optimisation problem exist. In the figure, this is indicated by

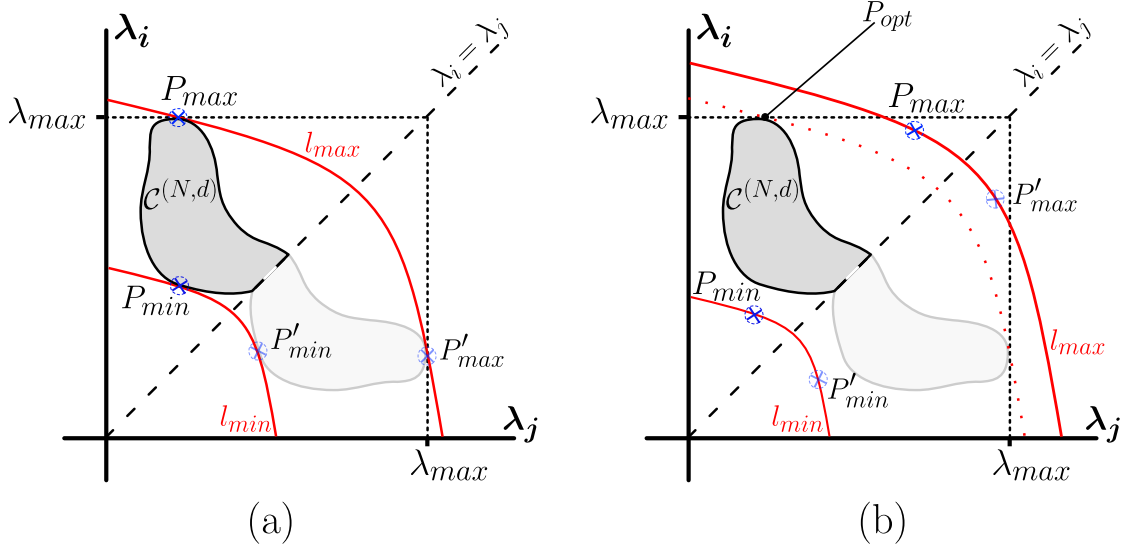


Figure 4.4: Schematic illustration of constrained optimisation within the ‘ λ_{max} -cube’ (indicated by the partially dotted black framed square): The dark grey set within the cube represents the set $\mathcal{C}^{(N,d)}$. The points P_{max} and P_{min} (blue reticles) mark positions of the global maximum and minimum of $tr(\rho^m)$. The red solid curves represent the constraining hyperplanes l_{max} and l_{min} . In (a), the variation yields optimal bounds; in (b) the variation yields non-optimal bounds. The optimal upper bound in (b) is indicated by the red dotted curve. For more details see text.

the mirrored light gray set and the points P'_{max} and P'_{min} . Instead of implementing the ordering constraints $\lambda_{i+1} \leq \lambda_i$ (marked by the 45°-dashed line) in the variation of $tr(\rho^m)$, one therefore may more easily select the solutions with ordered spectra as this will obviously yield the same constraining hyperplanes l_{max} and l_{min} . Notice that most of the points in l_{max} and l_{min} are not extremal points of the variation since they do not have the correct normalisation. Eventually, the outer approximation of $\mathcal{C}^{(N,d)}$ will of course be given by the intersection of all d conditions derived by the variation of the traces of $\rho^m, \forall m = 1 \dots d$.

Secondly, if the global maximum of $tr(\rho^m)$ within the λ_{max} -cube is *not* attained at a point of $\mathcal{C}^{(N,d)}$, then the constraint $tr(\rho^m) \leq tr(\rho^m)|_{P_{max}}$ will still exclude areas of common bosonic spectra and provide a restrictive necessary condition for N -representability. As a caveat, it is not the optimal bound that would be achieved by the (practically infeasible) variation over the domain of $\mathcal{C}^{(N,d)}$. This scenario is depicted in part (b) of Fig. 4.4, where the optimal bound is indicated by the curved red dotted line. The optimal point P_{opt} will lie on the boundary of $\mathcal{C}^{(N,d)}$. Further notice that the global maximum and the global minimum are not necessarily to be associated with the same case (a or b) in Fig. 4.4.

Let us now perform the constrained optimisation of $\text{tr}(\rho^m)$. The normalisation constraint $\text{tr}(\rho) = N$ can be implemented via using the Lagrange multiplier τ ; the inequality constraints $\lambda_i \geq 0$ and $\lambda_{max} - \lambda_j \geq 0$ are built in using the strictly non-negative KKT multipliers μ_i and ν_i , respectively. We notice that the quasi-regularity of the constraints is guaranteed by their linearity (cf. appendix, Sec. D). The set of KKT-equations (cf. Eqs. (D.9)) then reads as:

$$m(\lambda_i)^{m-1} = \tau + \mu_i - \nu_i, \quad \forall i = 1 \dots d, \quad (4.88a)$$

$$\sum_{i=1}^d \lambda_i = N, \quad (4.88b)$$

$$\lambda_i \geq 0, \quad \forall i = 1 \dots d, \quad (4.88c)$$

$$\lambda_{max} - \lambda_j \geq 0, \quad \forall i = 1 \dots d, \quad (4.88d)$$

$$\mu_i \geq 0, \quad \forall i = 1 \dots d, \quad (4.88e)$$

$$\nu_i \geq 0, \quad \forall i = 1 \dots d, \quad (4.88f)$$

$$\mu_i \lambda_i = 0, \quad \forall i = 1 \dots d, \quad (4.88g)$$

$$\nu_i (\lambda_{max} - \lambda_i) = 0, \quad \forall i = 1 \dots d. \quad (4.88h)$$

Due to Eqs. (4.88e) and (4.88f), one has to examine four different cases for each index $i = 1 \dots d$. Let us define the sets of indices attributed to those four different cases as:

$$\begin{aligned} \text{C1: } c_1 &:= \{i | \mu_i > 0 \wedge \nu_i = 0\}; & \text{C2: } c_2 &:= \{i | \mu_i = 0 \wedge \nu_i > 0\}; \\ \text{C3: } c_3 &:= \{i | \mu_i = 0 \wedge \nu_i = 0\}; & \text{C4: } c_4 &:= \{i | \mu_i > 0 \wedge \nu_i > 0\}; \end{aligned} \quad (4.89)$$

Observe that case C4 is impossible to achieve due to Eqs. (4.88g) and (4.88h). Because of Eq. (4.88g) one finds that for indices accounted to case C1

$$\lambda_i = 0, \quad \forall i \in c_1. \quad (4.90)$$

Similarly, it follows from Eq. (4.88h) that the natural occupation numbers with indices of case C2 saturate the upper bound:

$$\lambda_i = \lambda_{max}, \quad \forall i \in c_2. \quad (4.91)$$

All λ_i with indices belonging to c_3 have the same value. This is a consequence of Eq. (4.88a). Due to the normalisation condition Eq. (4.88b) and the fact that $\lambda_{max} < N$ for $1 < N < d$, one can further conclude that their value must be non-zero:¹⁴

$$0 < \lambda_i = \text{const.} < \lambda_{max}, \quad \forall i \in c_3. \quad (4.92)$$

¹⁴Here, we neglect the trivial cases of $N = d$, $N = 1$.

The set of potential maximising or minimising points of the variation of $tr(\rho^m)$ over the λ_{max} -cube is given by all combinations of cases C1 to C3:

$$\vec{\lambda}_{extr.} = \left\{ \underbrace{\lambda_{max}, \dots, \lambda_{max}}_{|c_2|}, \underbrace{\left(\frac{N - |c_2|\lambda_{max}}{|c_3|} \right), \dots, \left(\frac{N - |c_2|\lambda_{max}}{|c_3|} \right)}_{|c_3|}, \underbrace{0, \dots, 0}_{|c_1|} \right\}. \quad (4.93)$$

Note that the normalisation condition Eq. (4.88b) has been used to determine the eigenvalues associated to case C3. For every specific setting, i.e. number of particles and sites, one may now compute the value of $tr(\rho^m)$ at all vectors of the finite set $\{\vec{\lambda}_{extr.}(|c_1|, |c_2|, |c_3|) : |c_1| + |c_2| + |c_3| = d\}$ and thereby determine the global maximum and minimum. Example results are presented in Table 4.3.

Note that the normalisation condition further implies that $\lambda_{max}|c_2| \leq N$. In systems with half or lesser filling the multiplicity of λ_{max} eigenvalues, $|c_2|$, can thus at most be one:

$$N - 1 < \frac{d}{2} \implies |c_2| \leq 1. \quad (4.94)$$

Analogous restrictions to the multiplicity of λ_{max} in $\vec{\lambda}_{extr.}$ (4.93) can also be found for larger fillings. By similar considerations one also finds that $|c_3| \geq 2$.

Let us now add a few comments about Table 4.3. For various settings (N, d) , hardcore boson limits on $tr(\rho^m)$ are derived by evaluation of $tr(\rho^m)$ at the $\vec{\lambda}$ -vectors in Eq. (4.93); the resulting values are compared with their counterparts for common bosons. Limits with hardcore boson N -representation, i.e. optimal bounds (cf. discussion above and Fig. 4.4), are marked by asterisks. For the settings $(2, 4)$, $(3, 4)$ and $(4, 5)$ optimal upper bounds are added in round brackets. These bounds were computed by adopting the methods presented in Sec. 4.4.1.1. Square brackets indicate the conjectured optimal bounds and correspond to the spectrum of the $|\lambda_N^{\lambda_{max}}\rangle$ state.

Observe that for arbitrary settings of hardcore bosons (N, d) , the extended variation over the λ_{max} -cube successfully gives rise to bounds on all $tr(\rho^m)$ that are stricter than for common bosons. For a couple of settings, however, these bounds are not yet optimal. This is a consequence of Thm. 4, which implies that solution points (4.93) with multiplicities of λ_{max} greater than one are not N -representable.

Even though the variation over the λ_{max} -cube yields the spectrum of $|\psi_N^{\lambda_{max}}\rangle$,

$$\vec{\lambda}(|\psi_N^{\lambda_{max}}\rangle) = \left(\lambda_{max}, \frac{N(N-1)}{d(d-1)}, \dots, \frac{N(N-1)}{d(d-1)} \right), \quad (4.95)$$

to be the extremal point within $\mathcal{C}^{(N,d)}$ with the largest value of $tr(\rho^m)$, it could in principle happen that on the restricted variation domain of $\mathcal{C}^{(N,d)}$ a different maximal

(N, d)	m	$\min[tr(\rho_{(b)}^m)]$	$\min[tr(\rho_{(hcb)}^m)]$	$\max[tr(\rho_{(hcb)}^m)]$	$\max[tr(\rho_{(b)}^m)]$
$(2, 4)$	2	1	1^*	$2^{1/2} (2^{1/3})$	4
	3	$1/2$	$1/2^*$	$3^{1/2} (3^{7/18})$	8
	4	$1/4$	$1/4^*$	$5^{1/8} (5^{7/108})$	16
$(3, 4)$	2	$2^{1/4}$	3^*	$4^{1/2} (3)$	9
	3	$1^{11/16}$	3^*	$6^{3/4} (3^{3/4})$	27
	4	$1^{17/64}$	3^*	$10^{1/8} (5^{1/4})$	81
$(3, 5)$	2	$14/5$	$14/5$	$4^{17/25} [3^{3/5}]$	9
	3	$12/25$	$12/25$	$7^{14/25} [5^{47/50}]$	27
	4	$81/125$	$81/125$	$12^{357/625} [10^{53/100}]$	81
	5	$243/625$	$243/625$	$21^{48/125} [18^{4527/5000}]$	243
$(4, 5)$	2	$3^{1/5}$	4^*	$8^{8/25} (4)$	16
	3	$2^{14/25}$	4^*	$17^{23/25} (4^{24/25})$	64
	4	$2^6/125$	4^*	$39^{457/625} (7^9/125)$	256
	5	$1^{399/625}$	4^*	$90^{14/125} (10^{498/625})$	1024
$(3, 6)$	2	$3/2$	$3/2$	$5 [4^{1/5}]$	9
	3	$3/4$	$3/4$	$9 [8^{1/25}]$	27
	4	$3/8$	$3/8$	$17 [16^{1/125}]$	81
	5	$3/16$	$3/16$	$33 [32^{1/625}]$	243
	6	$3/32$	$3/32$	$65 [64^{1/3125}]$	729
$(4, 6)$	2	$3^{1/5}$	$3^{1/5}$	$8 [4^{4/5}]$	16
	3	$3^{1/5}$	$3^{1/5}$	$16 [8^{8/25}]$	64
	4	$3^{1/5}$	$3^{1/5}$	$32 [16^{16/125}]$	256
	5	$3^{1/5}$	$3^{1/5}$	$64 [32^{32/625}]$	1048
	6	$3^{1/5}$	$3^{1/5}$	$128 [64^{64/3125}]$	4096

Table 4.3: Necessary conditions for N -representability of hardcore bosons. Third and fourth column: hardcore boson upper and lower bounds on $\max_{\tilde{\lambda} \in \mathcal{C}^{(N,d)}} (tr(\rho_{(hcb)}^m))$ and $\min_{\tilde{\lambda} \in \mathcal{C}^{(N,d)}} (tr(\rho_{(hcb)}^m))$, respectively, derived by variation over the extended domain of the λ_{max} -cube for various settings (N, d) . Asterisks indicate optimal bounds; optimal bounds found by variation over $\mathcal{C}^{(N,d)}$ are shown in round brackets. Conjectured optimal bounds associated with the spectrum of $|\psi_N^{\lambda_{max}}\rangle$ are given in square brackets. To allow for a comparison, the third and sixth column display corresponding bounds for common boson 1-RDOs, $\rho_{(b)}$. For more details see text.

value of $tr(\rho^m)$ was attained somewhere on the boundary of $\mathcal{C}^{(N,d)}$ (cf. Fig. 4.4). More formally:

$$\max_{\vec{\lambda} \in \mathcal{C}^{(N,d)}} (tr(\rho^m)) \in \left[tr(\rho^m)|_{spec(|\psi_N^{\lambda_{max}}\rangle)}, \max_{\vec{\lambda} \in [0, \lambda_{max}]^d} (tr(\rho^m)) \right]. \quad (4.96)$$

The optimal bounds for the setting (2, 4) found by optimisation over $\mathcal{C}^{(2,4)}$ and the equality constraint Eq.(4.80) for one-hole systems, on the other hand, suggest that within $\mathcal{C}^{(N,d)}$ the functionals $tr(\rho^m)$ generally *do* attain their maximal value at the spectrum of $|\psi_N^{\lambda_{max}}\rangle$. This prompts the following conjecture:

Conjecture 1 (Maximal values of $tr(\rho^m)$ within $\mathcal{C}^{(N,d)}$)

For any number of hardcore bosons N on d lattice sites, the maximal values of all $tr(\rho^m)$, $\forall m = 1 \dots d$, are simultaneously achieved at the $\vec{\lambda}$ -vector of the $|\psi_N^{\lambda_{max}}\rangle$ state (cf. Eq. (4.16)):

$$\max_{\vec{\lambda} \in \mathcal{C}^{(N,d)}} (tr(\rho^m)) = \left(\frac{N}{d} \right)^m ((d - N + 1)^m + (N - 1)^m (d - 1)^{1-m}). \quad (4.97)$$

Note that in comparison with the upper bounds of common bosons, the hardcore boson bounds derived by optimisation over the λ_{max} -cube lie close to the conjectured optima (cf. Tab. 4.3). The extended variation yields good results, especially for settings with $2N \approx d$.

How about the lower bounds of $tr(\rho^m)$? Here, the situation is more intricate and whether bounds are optimal depends on whether N, d are odd or even. For settings with even N and even d the lower bound of

$$\min_{\vec{\lambda} \in [0, \lambda_{max}]^d} (tr(\rho^m)) = d \left(\frac{N}{d} \right)^m \quad \text{at} \quad \vec{\lambda} = \left(\frac{N}{d}, \dots, \frac{N}{d} \right) \quad (4.98)$$

is N -representable by

$$|\psi\rangle = |1, \dots, N\rangle + |3, \dots, N, N+1, N+2\rangle + \dots \\ + |d-N+1, \dots, d\rangle + |d-N+3, \dots, d, 1, 2\rangle + \dots, \quad (4.99)$$

and thus optimal. In systems with odd numbers of particles or sites no analogous construction to represent $\vec{\lambda} = (N/d, \dots, N/d)$ by a pure state is known to the author. Again recalling the analytical result for one-hole systems, Eq. (4.80), one is prompted to conjecture that the optimal minimal bound for $tr(\rho^m)$ is attained at exactly that extremal point $\lambda_{extr.}$ (4.93) which is still N -representable.

Before turning to the study of sufficient conditions in the next section let us briefly summarise the main results on necessary conditions for the hardcore boson 1-body N -representability. For the set of compatible spectra $\mathcal{C}^{(N,d)}$, an outer approximation can

be given in terms of bounds on the traces of the first d powers of ρ . By applying techniques of constrained optimisation to an extended variation domain, one finds bounds on each $tr(\rho^m)$, which represent a severe restriction in the space of common bosons. The derived restrictions give rise to necessary conditions on the $\vec{\lambda}$ -vector:

$$\min(tr(\rho^m)) \leq (\lambda_1)^m + \dots + (\lambda_d)^m \leq \max(tr(\rho^m)), \quad \forall m = 1 \dots d. \quad (4.100)$$

Note that the upper bound lies in the interval defined in Eq. (4.96). Under the thermodynamic limit of fixed particle number N and large number of sites d it thus approaches the bound for common bosons $\sim N^d$, which means that the influence of the hardcore constraint vanishes.

For the set of 1-RDOs of mixed states, necessary conditions on the one-particle spectrum may be determined the same way as above, extremising all traces $tr(\rho^m)$ over the λ_{max} cube. Due to Thm. 4, this extended variation domain is also an outer approximation for spectra of mixed states. The solution set of potentially extremal points agrees with the $\vec{\lambda}$ -vectors in Eq. (4.93) and the same (perhaps not yet optimal) bounds on all $tr(\rho^m)$ are established.

4.4.2 Necessary and sufficient conditions for pure N -representability

In order to determine necessary and sufficient conditions, one has to implement further constraints into the variation of the $tr(\rho^m)$. Let us illustrate the construction idea at the $(N = 3, d = 4)$ setting. Parametrised expressions for $tr(\rho^2)$, $tr(\rho^3)$ and $tr(\rho^4)$ were derived in Sec. 4.4.1.1 (cf. Eq. (4.79)). Computing their maxima and minima yielded necessary conditions.

Since, however, it was not taken into account that the variation of $tr(\rho^4)$ would, in addition to the normalisation, be constrained by the value assumed by $tr(\rho^3)$, the resulting boundaries did not give rise to sufficient conditions. This caveat can be met by implementing another constraint into the variation of $tr(\rho^4)$; the altered action reads:

$$S'_4[A_i, \mu_1, \mu_2] := tr(\rho^4) - \mu_1(\sigma^{(2)} - 1) - \mu_2(tr(\rho^3) - \alpha). \quad (4.101)$$

Here, $\alpha \in [3, 15/4]$ is the value assumed by $tr(\rho^3)$ which is enforced by the Lagrange multiplier μ_2 . The Euler-Lagrange equations of the action S'_4 constitute a parameter α dependent system of multivariate polynomial equations in the expansion coefficients A_i and the Lagrange multipliers $\mu_{1/2}$. This system again can be solved by using an implementation of the Buchberger algorithm to the CAS Mathematica. Because the

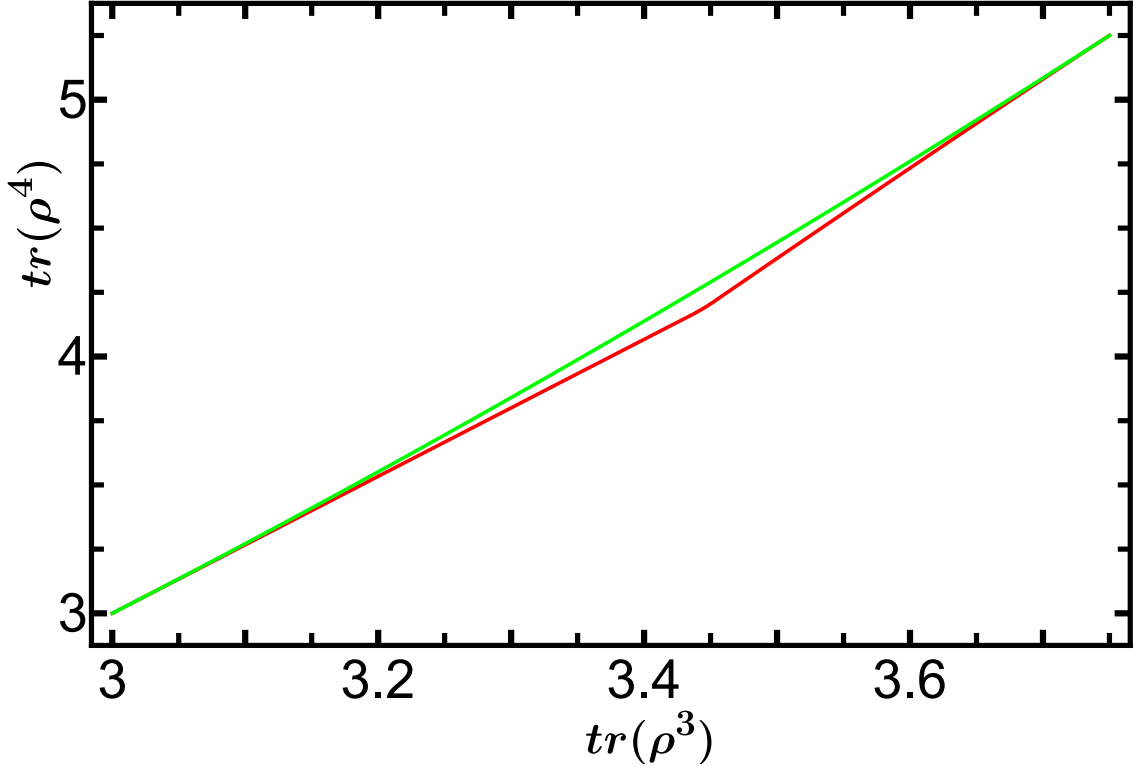


Figure 4.5: Set of compatible points in the $tr(\rho^3)$ - $tr(\rho^4)$ -plane of the $(N = 3, d = 4)$ hardcore boson setting. The upper bound $f^{up}(tr(\rho^3))$ is marked by the red line, the lower bound $f^{low}(tr(\rho^3))$ is marked by the green line.

solution set comprises more than 300 potential extremal points (A_i, μ_1, μ_2) it cannot be displayed here. By a careful evaluation of the action at all those points, one finds piecewise-defined analytical functions of the parameter α as upper and lower bounds on $tr(\rho^4)$:

$$f^{low}(tr(\rho^3) = \alpha) \leq tr(\rho^4) \leq f^{up}(tr(\rho^3) = \alpha). \quad (4.102)$$

Both functions are plotted in Fig. 4.5. They surround the area of compatible points in the $tr(\rho^3)$ - $tr(\rho^4)$ -plane and give rise to necessary and sufficient conditions for N -representability of $N = 3$ hardcore bosons on $d = 4$ lattice sites:

$$\begin{aligned} \lambda_1 + \lambda_2 + \lambda_3 + \lambda_4 &= 3, \quad (\lambda_1)^2 + (\lambda_2)^2 + (\lambda_3)^2 + (\lambda_4)^2 = 3, \\ 3 &\leq (\lambda_1)^3 + (\lambda_2)^3 + (\lambda_3)^3 + (\lambda_4)^3 \leq 3^{3/4}, \\ f^{low}\left(\sum_i (\lambda_i)^3 = \alpha\right) &\leq (\lambda_1)^4 + (\lambda_2)^4 + (\lambda_3)^4 + (\lambda_4)^4 \leq f^{up}\left(\sum_i (\lambda_i)^3 = \alpha\right). \end{aligned} \quad (4.103)$$

Note that instead of modifying the action S_4 by including a constraint on the value of $tr(\rho^3)$, one equivalently could have modified S_3 by implementing a constraint on the

value of $\text{tr}(\rho^4)$. Both modified actions give rise to structurally similar Euler-Lagrange equations and their solutions are found to coincide.

Although the above scheme can in principle be extended and applied to arbitrary settings (N, d) one cannot expect the arising systems of multivariate polynomial equations to be analytically solvable. The original problem of determining the set of roots of the characteristic polynomials of all parametrised 1-RDOs is converted into a system of multivariate polynomial equations in the expansion coefficients of the N -particle state. This approach may prove helpful in future investigations on the complexity class of the hardcore boson N -representability problem.

4.5 Bounds on one-particle entropy measures

One-particle entropies of many-body quantum states ρ_N are important measures of the information contained in reduced one-particle states about an N -particle state. Several types of entropy functions S have been suggested in the past [80, 98, 13], offering different characteristics and advantages. Though considered not to be actual observables due to their non-linear dependence on ρ , (quantum) entropic measures on density operators, encompassing 1-RDOs, were found to play a key role in many branches of physics, such as generalised uncertainty relations [66, 103, 110], quantum transport and diffusion processes [65, 31, 72, 3], and many others.

In this section, we are going to discuss the behaviour of three different one-particle entropy measures in systems of hardcore bosons: the Rényi entropy, the Tsallis entropy and the Shannon entropy. In the present section, the 1-RDO will be normalised to one, i.e. $\text{tr}[\rho_1] = 1$. Consequently, the maximal occupation number reads $\lambda_{max} = (d - N + 1)/d$.

It is well known that one-particle entropies of N common bosons can reach zero since all particles may populate the same one-particle state. For fermions the Pauli exclusion principle (cf. 2.2, Eq. (2.26)) prevents this and leads to strictly positive lower one-particle entropy bounds. Although specific to a particular basis, hardcore bosons also obey a form of an exclusion principle (cf. Eq. (4.5)). This raises the interesting question of which mechanism - particle statistics or physical exclusion principle - will dominate in the establishment of the lower one-particle entropy bound for hardcore bosons.

Rényi entropy

The Rényi entropy is defined via [80, 13]:

$$R_\alpha(\rho) = \frac{1}{1-\alpha} \ln \left(\text{tr}(\rho^\alpha) \right), \quad \alpha \in [0, +\infty]. \quad (4.104)$$

It is a non-increasing function in α , i.e. $R_\alpha(\rho) \geq R_{\alpha'}(\rho)$ if $\alpha \leq \alpha'$ (see, e.g., Ref. [6], chapter 5). In particular, one finds¹⁵

$$R_0 \geq R_1 \geq R_2 \geq R_\infty. \quad (4.105)$$

The limit $\lim_{\alpha \rightarrow 1} R_\alpha$ retrieves the Shannon entropy, which is going to be examined further below. R_0 , R_2 and R_∞ are known as the Hartley, Collision and min-entropy, respectively.

The minimal value of all 1-RDO Rényi entropies in systems of N common bosons on d lattice sites becomes 0. For Fermions one finds $\min(R_\alpha) = \ln(N)$. The question is: what are the respective general limitations for hardcore bosons?

The min-entropy of $\rho_1^{(hcb)}$ assumes its smallest value at the $|\psi_N^{\lambda_{max}}\rangle$ state:

$$\min(R_\infty) = -\ln \left(\max_i (\lambda_i) \right) = \ln(d) - \ln(d - N + 1) \leq \ln(N), \quad (4.106)$$

with equality only for $N = 1, d$. This value is smaller than for fermionic systems but nevertheless strictly non-zero for $N > 1$. Rényi entropies for $1 < \alpha < \infty$ attain their minimal value at the maximum of $\text{tr}(\rho^\alpha)$. The upper bounds for this quantity have been studied in the previous section and possible values have been confined to the interval given in Eq. (4.96). Note that this interval still has to be rescaled by $(\text{tr}(\rho_1))^{-\alpha}$ to match the normalisation condition of $\text{tr}(\rho_1) = 1$. For finite numbers of particles and sites, the entropies are strictly positive, which may also be seen as an immediate consequence of the inequalities (4.105) and Eq. (4.106). The minimal values of R_α , $1 < \alpha < \infty$, are bounded from above by the one-particle entropy of the $|\psi_N^{\lambda_{max}}\rangle$ state:

$$0 < \min(R_\alpha) \leq \frac{1}{1-\alpha} \ln \left(\left(\frac{d-N+1}{d} \right)^\alpha + (d-1) \left(\frac{N-1}{d(d-1)} \right)^\alpha \right) \leq \ln(N). \quad (4.107)$$

The last inequality is strict for all $N < d$ if $\alpha > 2$, which may be verified by examining the functional form of the bounding term with respect to N and α ; if Conj. 1 should be confirmed, the second inequality would become an equality.

¹⁵The second inequality may quickly be seen as a consequence of Jensen's inequality: Let f be a real-valued convex function in one variable. For $\vec{x}, \vec{a} \in \mathbb{R}^d$ and $a_i \geq 0$ and $\sum_i a_i = 1$ the following inequality holds: $f(a_1 x_1 + \dots + a_d x_d) \leq a_1 f(x_1) + \dots + a_d f(x_d)$; (cf. Ref. [43]).

Furthermore, the relations (4.106) and (4.107) allow for the computation of the thermodynamic limit of the lower bound of R_α , $\alpha > 1$, under constant particle number:

$$\lim_{d \rightarrow \infty} \left(\min (R_\alpha(\rho_1^{(hcb)})) \right) \Big|_N = 0. \quad (4.108)$$

The influence of the hardcore constraint diminishes and the lower bound approaches the value of common bosons.

At this point, let us add a remark on the Collision entropy of one-hole systems. By invoking the general constraint Eq. (4.80) on hardcore systems with $N = d - 1$ particles in a pure state one gets:

$$R_2(\rho_1^{(N=d-1)}) = \ln(N). \quad (4.109)$$

The Collision entropy has the same constant value for all pure states. Firstly note that since the set of all 1-RDOs is a convex set (cf. Eq. (4.7)) and R_2 is a concave function, the minimum of $R_2(\rho_1^{(N=d-1)})$ will be achieved at a pure state, making the rhs in Eq. (4.109) the lower bound also under inclusion of mixed states. Secondly, this result agrees with the upper bound on $\min(R_\alpha)$ in relation (4.107) when substituting d by $N + 1$, which further supports Conj. 1. Thirdly, notice that the result does not contradict the thermodynamic limit (4.108) since N depends on d .

Lastly, we observe that the $|\psi_N^{\lambda_{max}}\rangle$ state surprisingly maximises the Hartley entropy. Numerical investigations suggest that the minimum of the Hartley entropy is achieved at states of single permanents, though an analytical result remains an objective of future research.

Tsallis entropy

The Tsallis entropy can be written as [98, 13]:

$$T_\alpha(\rho) = \frac{1}{1 - \alpha} \left(\text{tr}(\rho^\alpha) - 1 \right). \quad (4.110)$$

In the limit of α approaching unity, the Tsallis entropy reduces to the von Neumann entropy. After its introduction by Tsallis in 1988, it was initially challenged because of its non-additivity. The occurrence of Tsallis statistics in the description and experimental observation of a number of physical systems thus came as a surprise. Here, the motion of ultracold atoms in optical lattices presents an important example relevant to this thesis [65, 31]. Constraints on T that arise from the hardcore property may lead to restrictions on the transport mechanisms. This motivates a closer look.

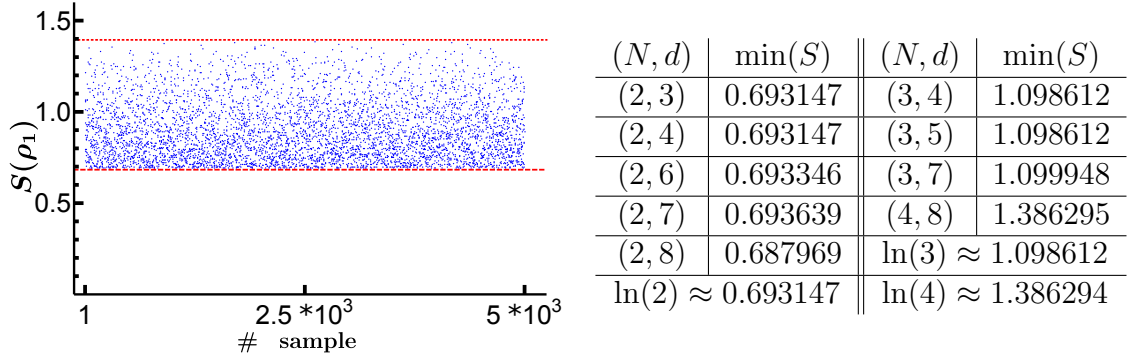


Figure 4.6: Estimates of the lower one-particle von Neumann entropy bound $\min(S)$, derived by sampling of generic hardcore boson states. Left: graphical display of sampling convergence for $N = 2$ particles on $d = 4$ sites. Right: Selected minimal sampled entropy values.

For $\alpha > 1$, the minimal Tsallis entropy of N common Bosons on d sites is given by 0, for fermions it becomes $(\alpha - 1)^{-1}(1 - N^{1-\alpha})$. The bounds of the Tsallis entropy for $\alpha > 1$ linearly depend on the bounds of $\text{tr}(\rho^m)$ determined in Sec. 4.4.1. For finite number of sites and particles, the lower bound is strictly postive and bounded from above by the one-particle entropy of the $|\psi_N^{\lambda_{max}}\rangle$ state.

For $\alpha < -1$, the smallest one-particle Tsallis entropy is achieved by the totally mixed state with all $\lambda_i = 1/d$.

As for Rényi entropies, a special conclusion can be drawn for pure one-hole states and $\alpha = 2$. Using the equality constraint Eq. (4.80) one finds:

$$T_2(\rho_1^{(N+1=d)}) = 0. \quad (4.111)$$

von Neumann entropy

Most commonly encountered, the von Neumann entropy [101] is defined via:

$$S = -\text{tr}(\rho \ln(\rho)). \quad (4.112)$$

In systems of common bosons the lower bound of this one-particle entropy is zero and for N fermions it is given by $\ln(N)$.

For $N = d$ hardcore bosons, the one-particle entropy is trivially given by $\ln(N)$. For $1 < N < d$, the maximal occupation number was shown to exceed one, which suggests that the lower bound of $S(\rho_1^{(hcb)})$ might be smaller than the fermionic bound. The numerical results of randomly sampled generic quantum states thus come as a surprise since they indicate a lower bound of $\ln(N)$ for a number of settings (N, d) . A selection of these results is shown in Fig. 4.6. Observe that $\ln(N)$ cannot be the

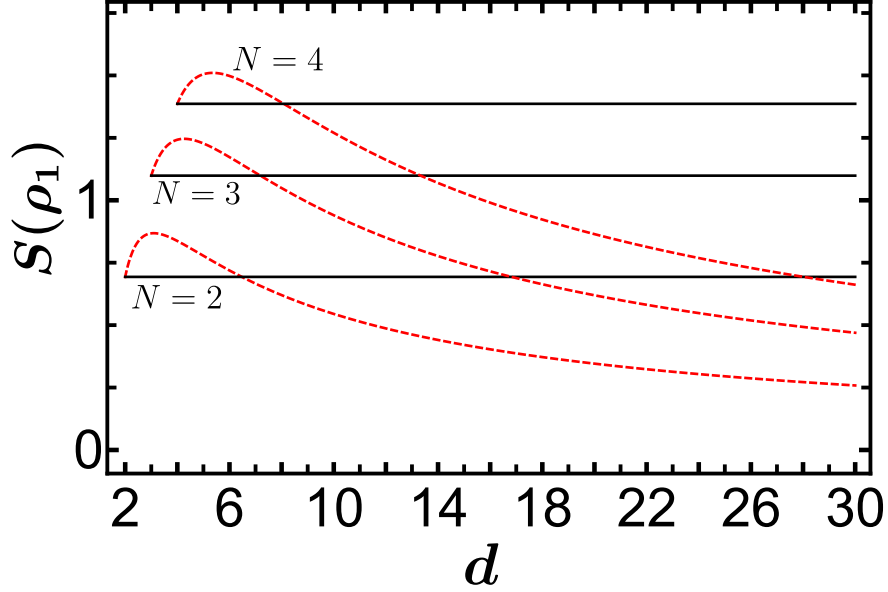


Figure 4.7: One-particle von Neumann entropies of single permanent (black, solid) and $|\psi_N^{\lambda_{max}}\rangle$ states (red, dashed) for particle numbers $N = 2, 3, 4$ as a function of the number of sites d (cf. Eq. (4.114)). For more details see text.

general lower entropy bound for hardcore bosons because - alongside other reasons - a smaller value has numerically been found for the $(2, 8)$ setting. Nevertheless, it is possible to derive the lower bound for one-hole systems by using the inequality for Rényi entropies (4.105) and the lower bound for the Collision entropy R_2 (4.109):

$$\min(S)|_{N=d-1} = \ln(N). \quad (4.113)$$

The one-particle entropy attains this limit for any state comprising of a single hardcore permanent $|i_1, \dots, i_N\rangle$.

What happens if one increases the number of sites while keeping N constant? We know that for increasing d the maximal occupation number converges to one and therefore a single-particle state can be macroscopically occupied. Consequently, the one-particle entropy should converge to zero. Fig. 4.7 graphically illustrates this fact by displaying the von Neumann entropies of a single permanent and the $|\psi_N^{\lambda_{max}}\rangle$ state. The latter one is given by:

$$S(\rho_1)|_{|\psi_N^{\lambda_{max}}\rangle}(N, d) \equiv S^{(\lambda_{max})} = \frac{(d - N + 1)}{d} \ln\left(\frac{d}{d - N + 1}\right) + \frac{N - 1}{d} \ln\left(\frac{d(d - 1)}{N - 1}\right). \quad (4.114)$$

Regarded as a function of d for fixed N it is larger than $\ln(N)$ in the neighbourhood of $N \approx d$. However, when d increases further the entropy of the $|\psi_N^{\lambda_{max}}\rangle$ state falls

below $\ln(N)$ and, as expected, converges to zero:

$$\lim_{d \rightarrow \infty} \left(S^{(\lambda_{max})} \right) \Big|_N = 0. \quad (4.115)$$

Note that no analytical expression for the intersection points $\tilde{d}$, $S^{(\lambda_{max})}(\tilde{d}) = \ln(N)$, can be given since the defining equation is transcendental. Numerical solutions for $10 \leq N \leq 10^{60}$ suggest that $S^{(\lambda_{max})}(d) < \ln(N)$ for $d \geq \tilde{d} = N + 4$.

In order to analytically derive the general form of the lower bound of S for hardcore bosons, one has to evaluate the following expression:

$$\min_{\vec{\lambda} \in \mathcal{C}^{(N,d)}} \left(- \sum_{i=1}^d \lambda_i \ln(\lambda_i) \right). \quad (4.116)$$

This is a challenging task since no feasible expression of $\mathcal{C}^{(N,d)}$ is yet known. Let us now recall the techniques used in Sec. 4.4.1.2. By extending the domain of optimisation to the λ_{max} -cube and using the KKT-formalism, one gets a system of necessary conditions on $\vec{\lambda}$ -vectors at potential minima:

$$-\ln(\lambda_i) - 1 = \tau + \mu_i - \nu_i, \quad \forall i = 1 \dots d, \quad (4.117a)$$

$$\sum_{i=1}^d \lambda_i = 1, \quad (4.117b)$$

$$\lambda_i \geq 0, \quad \forall i = 1 \dots d, \quad (4.117c)$$

$$\lambda_{max} - \lambda_j \geq 0, \quad \forall j = 1 \dots d, \quad (4.117d)$$

$$\mu_i \geq 0, \quad \forall i = 1 \dots d, \quad (4.117e)$$

$$\nu_i \geq 0, \quad \forall i = 1 \dots d, \quad (4.117f)$$

$$\mu_i \lambda_i = 0, \quad \forall i = 1 \dots d, \quad (4.117g)$$

$$\nu_i (\lambda_{max} - \lambda_i) = 0, \quad \forall i = 1 \dots d. \quad (4.117h)$$

Here, τ is a Lagrange multiplier enforcing the normalisation constraint Eq. (4.117b). The KKT multipliers μ_i and ν_i are strictly positive. As well as $\text{tr}(\rho^m)$, the von Neumann entropy function is symmetric in all λ_i . By a similar line of reasoning as in Sec. 4.4.1.2, the solutions therefore take a form as given in Eq. (4.93). In order to determine the global minimum within the λ_{max} -cube, one has to evaluate the von Neumann entropy at a finite number of solutions, Eq. (4.93), taking into account the normalisation condition. For $d > 2N - 1$, the multiplicity of λ_{max} in $\vec{\lambda}_{extr.}$ (4.93) is at most one (4.94), consequently:

$$\min_{\vec{\lambda} \in \mathcal{C}^{(N,d)}} (S) \in \left[\frac{d - N + 1}{d} \ln \left(\frac{d}{d - N + 1} \right) + \frac{N - 1}{d} \ln \left(\frac{d}{N - 1} \right), S^{(\lambda_{max})} \right] \quad (4.118)$$

Notice that the lower bound is strictly positive but converges to zero in the limit of large numbers of sites and constant particle numbers.

To summarise, analytical (for one-hole systems) and numerical evidence suggests that the lower bound on the one-particle von Neumann entropy of hardcore bosons on ‘small’ Hilbert spaces ($d - N \leq 3$) resembles the fermionic limit of $\ln(N)$. When the size of $\mathcal{H}_1^{(d)}$ is increased, the macroscopic population of a single-particle state becomes possible and the lower bound on the one-particle entropy approaches the bosonic value in the thermodynamic limit. This observation supports the notion of the hybrid character of hardcore bosons and is a direct witness of the competition between particle statistics and the physical lattice based exclusion principle.

In the next section, we are going to examine Hamiltonians whose ground states saturate the occupation number constraint.

4.6 Pinning of hardcore boson states

So far, we have investigated various ways to characterise the set of compatible one-particle spectra $\mathcal{C}^{(N,d)}$ of hardcore bosons. According to the introductory remarks on minimisation of the energy functional (cf. Fig. 4.1) in systems which only encompass 2-body interactions in form of the hardcore type, the respective $\vec{\lambda}$ -vector of the ground state is pinned to the boundary of $\mathcal{C}(N, d)$. In this section, we shall present two physical systems in which the saturation of constraints becomes explicit.

At first, the ground state of N bosons on a star lattice will be analytically derived. It will be demonstrated that a projective measurement on the central site of the star lattice will allow one to engineer the $|\psi_N^{\lambda_{max}}\rangle$ state on a one-dimensional ring of lattice sites. Originally, this lattice type was proposed by van Dongen et al. in Ref. [99] and investigated for spinful fermionic particles. More recently, Vidal et al. [100] have described the behaviour of non-interacting bosons on the star lattice. The results for hardcore bosons here emphasise their hybrid character.

The second model system to be considered is the 1D quantum lattice gas, which was firstly studied by Matsubara and Matsuma [67]. Despite additional 2-body interaction terms beyond the hardcore interaction, the ground state is found to be the $|\psi_N^{\lambda_{max}}\rangle$ state. This is a remarkable aspect of the model since energy minimisation of Hamiltonians comprising arbitrary 2-body terms generally only enforces pinning on the 2-RDO level. Finally, a route to explore *quasi*-pinning of hardcore bosons will be proposed.

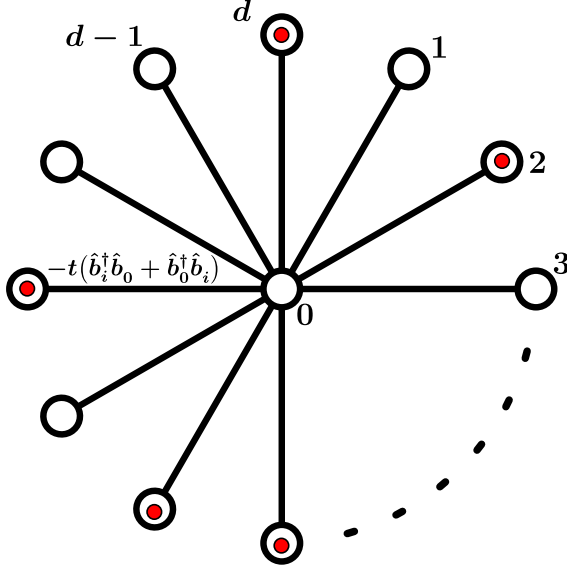


Figure 4.8: The (bosonic) Hubbard Star model. Only hopping between the outer sites 1 to d and the centre site 0 is permitted (see text for more details).

4.6.1 The Hubbard Star

Consider a lattice with sites 1 to d located on a circle and site 0 placed in the center of the circle (cf. Fig. 4.8). Further assume that tunneling between different sites on the outer circle is suppressed. The particles, however, may tunnel between the ring sites and the central site at a rate of t . The corresponding terms in the Hamiltonian read $-t(\hat{b}_i^\dagger \hat{b}_0 + \hat{b}_0^\dagger \hat{b}_i)$. In order to describe hardcore bosons, one has to project these operators to the hardcore boson Hilbert space $\mathcal{H}_N^{(hcb)}$ (cf. Eq. (4.9) and, e.g., Ref. [62]). The resulting Hamiltonian is given by:

$$\hat{H} = -t \sum_{i=1}^d \hat{b}_0^\dagger \sqrt{(1 - \hat{n}_0)} \sqrt{(1 - \hat{n}_i)} \hat{b}_i + h.c., \quad (4.119)$$

where as usual $\hat{n}_k = \hat{b}_k^\dagger \hat{b}_k$ represents the number operator. The Hamiltonian conserves the total particle number, i.e. $[\hat{H}, \sum_{i=0}^d \hat{n}_i] = 0$, and therefore the restriction to a Hilbert space with fixed particle number is justified. The model shall be called the *(bosonic) Hubbard star*.

In order to determine the ground state of the Hamiltonian it proves helpful to apply the spin- $\frac{1}{2}$ Holstein-Primakoff transformation [40]:

$$\hat{S}_j^+ = \sqrt{1 - \hat{n}_j} \hat{b}_j, \quad \hat{S}_j^- = \hat{b}_j^\dagger \sqrt{1 - \hat{n}_j}, \quad \hat{S}_j^z = \frac{1}{2} - \hat{n}_j, \quad \forall j = 0 \dots d. \quad (4.120)$$

The new observables $\hat{\mathbf{S}}_j$ are well known to form a spin-algebra:

$$[\hat{S}_i^+, \hat{S}_j^-] = 2\delta_{ij} \hat{S}_j^z, \quad [\hat{S}_i^z, \hat{S}_j^\pm] = \pm \delta_{ij} \hat{S}_j^\pm. \quad (4.121)$$

The transformed Hamiltonian reads:

$$\hat{H}' = -t \sum_{i=1}^d \hat{S}_0^+ \hat{S}_i^- + \hat{S}_0^- \hat{S}_i^+. \quad (4.122)$$

It acts on the Hilbert space $\mathbb{C}^{2(d+1)}$. Note that the vacuum state of the original Fock space is transformed into the full-spin-up polarised state $|\uparrow_0, \dots, \uparrow_d\rangle$ and that the creation of a hardcore boson corresponds to a spin flip. Consequently, N -particle states are mapped to states with total magnetic quantum number $m_{tot} = d/2 - N$, i.e.

$$\left(\sum_{i=0}^d \hat{S}_i^z \right) |\psi\rangle = \left(\frac{d}{2} - N \right) |\psi\rangle. \quad (4.123)$$

In the next step, one introduces the total spin operator on the ring, $\mathbf{S}_R = \sum_{i=1}^d \mathbf{S}_i$, which simplifies the Hamiltonian further :

$$\hat{H}' = -t(S_0^+ S_R^- + S_0^- S_R^+). \quad (4.124)$$

Without loss of generality, one may use the ansatz:

$$|\psi\rangle = \alpha |\uparrow_0\rangle \otimes |\psi_A\rangle + \beta |\downarrow_0\rangle \otimes |\psi_B\rangle, \quad (4.125)$$

and evaluate the Schrödinger equation. By sorting terms with respect to the spin basis $\{|\uparrow_0\rangle, |\downarrow_0\rangle\}$ one gets:

$$\begin{aligned} E\alpha |\psi_A\rangle &= -t\beta S_R^- |\psi_B\rangle, \\ E\beta |\psi_B\rangle &= -t\alpha S_R^+ |\psi_A\rangle. \end{aligned} \quad (4.126)$$

Here, E represents the energy eigenvalue. Normalisation of the ansatz state (4.125) requires $|\alpha|^2 + |\beta|^2 = 1$ if one assumes that the states $|\psi_{A/B}\rangle$ are normalised to unity. Since at this point we are interested in the ground state of the Hubbard star, we only consider solutions with negative energy E . Then Eqs. (4.126) imply that $\alpha, \beta \neq 0$. Both equations may easily be decoupled:

$$\begin{aligned} E^2 \alpha |\psi_A\rangle &= t^2 \alpha S_R^- S_R^+ |\psi_A\rangle, \\ E^2 \beta |\psi_B\rangle &= t^2 \beta S_R^+ S_R^- |\psi_B\rangle. \end{aligned} \quad (4.127)$$

Recall that for spin states the solution to the second equation is given by elements of the simultaneous eigenstate basis of $\mathbf{S}_R^2$ and S_R^z , which may be labelled by the respective eigenvalues s_R and m_R :

$$S_R^+ S_R^- |s_R, m_R\rangle = ((s_R(s_R + 1) - m_R(m_R - 1)) |s_R, m_R\rangle. \quad (4.128)$$

The lowest (negative) energy eigenvalue E is achieved when E^2 becomes maximal and thus one has to determine the maximal prefactor of the rhs in Eq. (4.128). Due to Eqs. (4.123) and (4.125), the magnetic quantum number of $|\psi_B\rangle$ is fixed by $m_R = d/2 - (N - 1)$. Therefore, the maximal value of E^2 is attained at the spin eigenstate with $s_R = d/2$ and the ground state energy E_0 becomes:

$$E_0 = -|t|\sqrt{N(d - N + 1)}. \quad (4.129)$$

Up to normalisation, the explicit form of the spin eigenstate $|s, m\rangle$ may be derived by successive action of the ladder operators on fully polarised states:

$$|\psi_B\rangle \propto |s_R = \frac{d}{2}, m_R = \frac{d}{2} - (N - 1)\rangle \propto (S_R^-)^{(N-1)} |\uparrow_1, \dots, \uparrow_d\rangle. \quad (4.130)$$

Substitution into Eq. (4.126) allows one to determine the coefficients α and β , and express the ground state of the Hubbard star in the spin basis:

$$|\psi\rangle = \frac{1}{\sqrt{2\binom{d}{N}}}(S_R^-)^N |\uparrow_0, \uparrow_1, \dots, \uparrow_d\rangle + \frac{1}{\sqrt{2\binom{d}{N-1}}}(S_R^-)^{N-1} |\downarrow_0, \uparrow_1, \dots, \uparrow_d\rangle \quad (4.131)$$

By using the inverse Holstein-Primakoff transformation, this state may be mapped back to the hardcore boson Hilbert space. To summarise, the hardcore boson ground state and energy are given by:

$$|\psi\rangle = \frac{1}{\sqrt{2}} |\psi_{R,N}^{\lambda_{max}}\rangle + \frac{1}{\sqrt{2}} \hat{b}_0^\dagger |\psi_{R,N-1}^{\lambda_{max}}\rangle, \quad E_0 = -|t|\sqrt{N(d - N + 1)}. \quad (4.132)$$

Here, $|\psi_{R,N}^{\lambda_{max}}\rangle$ denotes the state of maximal occupation number (4.16) of N particles on d sites of the ring. Note that the ground state alternatively could have been derived by using an ansatz state in $\mathcal{H}_N^{(hcb)}$ similar to (4.125). The expansion coefficients of this state may then be determined by a straightforward but tedious evaluation of the Schrödinger equation and the ground state energy may be computed by considering $\langle \hat{H} \rangle$ as a functional of the expansion coefficients.

The result shows that the ground state of hardcore bosons on a Hubbard star lattice does generally not assume the form of the $|\psi_N^{\lambda_{max}}\rangle$ state of N particles on $(d + 1)$ sites.¹⁶ However, if one carries out a projective measurement on the occupation number of the central site (e.g. by using a laser probe beam), then the resulting state on the outer ring is indeed a $|\psi^{\lambda_{max}}\rangle$ state and may be preserved by means of continuing measurements and the quantum Zeno effect (see, e.g., Ref. [33]). The system's state saturates the $\lambda_1 \leq \lambda_{max}$ constraint and is exactly pinned to the boundary of

¹⁶An exception is given by $N = 2$ and $d = 3$.

$\mathcal{C}^{(N,d)}$. For smaller filling factors N/d , a large fraction of the bosons condensates into the zeroth Bloch state of the ring. Recall that due to the structure of the 1-RDO (cf. Eq. (4.54)), the projected ground state further exhibits off-diagonal long-range order $\langle \hat{b}_j^\dagger \hat{b}_k \rangle$ and 2-body correlations (4.59), which do not vanish in the thermodynamic limit. Together, these properties are commonly considered as the defining criteria of a Bose-Einstein condensate [28, 107].

Further observe that the Hubbard star Hamiltonian for hardcore bosons is structurally different from its fermionic counterpart. More specifically, by applying the Jordan-Wigner transformation [45] of the spin operators

$$S_i^- = \prod_{j<i} (1 - 2\hat{c}_j^\dagger \hat{c}_j) \hat{c}_i^\dagger, \quad S_i^+ = \prod_{j<i} (1 - 2\hat{c}_j^\dagger \hat{c}_j) \hat{c}_i, \quad (4.133)$$

to the Hamiltonian (4.122), one yields:

$$\hat{H} = +t\hat{c}_0\hat{c}_1^\dagger + t \sum_{i=2}^d \left((1 - 2\hat{c}_1^\dagger \hat{c}_1) \dots (1 - 2\hat{c}_{i-1}^\dagger \hat{c}_{i-1}) \hat{c}_0 \hat{c}_i^\dagger \right) + h.c. \quad (4.134)$$

By contrast, the Hubbard star Hamiltonian for spinless fermions reads:

$$\hat{H} = -t \sum_{i=1}^d \hat{c}_0 \hat{c}_i^\dagger + h.c. \quad (4.135)$$

A thorough investigation of the spectrum and a comparison with the hardcore boson Hubbard star will be an objective of future research.¹⁷

Last but not least, we mention that the ground state of non-interacting bosons on the Hubbard star lattice was derived by Vidal et al. [100]:

$$|\bar{\psi}\rangle = \left(\frac{1}{\sqrt{2}} \hat{b}_0^\dagger + \frac{1}{\sqrt{2d}} \sum_{i=1}^d \hat{b}_i^\dagger \right)^N |\rangle. \quad (4.136)$$

Observe that, intriguingly, due to Eq. (4.67), the projection of this state onto the hardcore boson Hilbert space exactly reproduces the ground state for hardcore bosons, derived above (4.132), up to a normalisation factor. The question whether this relation also holds for more general types of lattices is still open and remains an objective of future research.

¹⁷Note that in the work of van Dongen et al. the ground state has only been derived for spinful fermions in the half-filled case.

4.6.2 1D quantum lattice gas

The pinning of the Hubbard star ground state (4.132) may be seen as a natural consequence of the Hamiltonian only comprising 2-body terms in form of the on-site interaction (recall introductory discussion and Fig. 4.1). The ground state of Hamiltonians encompassing further 2-body terms can *not* generally be expected to be pinned on the boundary of $\mathcal{C}^{(N,d)}$. Interestingly, for specific parameters the ground state of the so-called *1D quantum lattice gas* becomes the $|\psi_N^{\lambda_{max}}\rangle$ state despite of additional 2-body interaction terms present in the Hamiltonian. The model, originally proposed by Matsubara and Matsuda [67], considers a hardcore boson system with hopping between neighbouring sites and attractive nearest-neighbour interactions:

$$\hat{H} = -t \sum_{i=1}^d \left(\hat{b}_i^\dagger \hat{b}_{i+1} + h.c. \right) - V \sum_{i=1}^d \hat{n}_i \hat{n}_{i+1} + \frac{U}{2} \sum_{i=1}^d \hat{n}_i (\hat{n}_i - 1) \quad (4.137)$$

If one projects this Hamiltonian to $\mathcal{H}_N^{(hcb)}$ and applies the Holstein-Primakoff transformation, one derives the Heisenberg XXZ model:

$$\hat{H}' = -2t \sum_{i=1}^d \left(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y \right) - V \sum_{i=1}^d S_i^z S_{i+1}^z. \quad (4.138)$$

For $V = 2t$, the Hamiltonian reduces to $\sum_i \mathbf{S}_i \cdot \mathbf{S}_{i+1}$. The expectation value of each of these terms becomes minimal if the quantum state is symmetric in both corresponding spins and therefore the ground state is seen to be the $|\psi_N^{\lambda_{max}}\rangle$ state.

The model further provides an ideal testing ground to explore quasipinning of hardcore boson states in future research. For specific settings (N, d) , one can compute the ground state of the Hamiltonian (4.138) for $V = 2 + \delta$ and subsequently determine its associated 1-RDO as a perturbation in δ . The quasipinning measured by $D(\epsilon) = \lambda_{max} - \lambda_1(\epsilon)$ can then be expressed as a function $D(\epsilon) = \mathcal{O}(\epsilon^2)$ in the perturbation parameter.

Chapter 5

Summary and conclusion

In this chapter, we summarise and discuss the main results and provide an outlook on possible objectives of future research.

In chapter 2, we have reviewed the concepts and notations of many-body quantum mechanics. This allowed us to present the r -body N -representability problem, which for $r \geq 2$ is found generally intractable [63]. The physical relevance of reduced particle information is a direct consequence of physical non-relativistic Hamiltonians only comprising 1- and 2-body terms. This significantly simplifies the corresponding energy functional (2.25) and opens the possibility for an efficient derivation of the respective ground state, provided a concise solution of the N -representability problem was found.

We have seen that the solution of the *pure* N -representability problem for fermionic one-particle reduced density operators (1-RDOs) is given by a set of linear inequalities on the eigenvalues (NONs) of the 1-RDO, called the Generalised Pauli constraints (GPCs) [1, 52]. They form tighter restrictions on the spectra of fermionic 1-RDOs than the Pauli exclusion principle, which itself provides a solution to the *mixed* 1-body N -representability problem. The Pauli exclusion principle gives rise to the Pauli hyper cube of compatible spectra of mixed states, whereas GPCs are related to a polytope $\mathcal{P}$ of compatible spectra within the hypercube.

One major aspect of the physical relevance of the GPCs is given by the pinning effect in which the NONs saturate some of the linear inequalities [52]. Pinning as an effect in the one-fermion picture comes with a remarkable structural simplification of the N -fermion wave function as it reduces the number of Slater determinants required in an expansion series. This surprising reversibility of extremal reduced particle information was also found to extend to the approximate saturation of GPCs, which is called the quasipinning effect [87, 84]. The quasipinning effect is a direct witness of the competition between energy minimisation and the antisymmetry of the

fermionic wave function. In order to study the origin and mechanism behind it, two measures have been reviewed.

The minimal distance D_{min} evaluates the l_1 distance of the $\vec{\lambda}$ -vector of NONs to the boundary of the polytope. It is an absolute measure, which also characterises the degree of structural simplification of the corresponding N -fermion wave function. Practical means of its computation have been introduced by the concept of a truncated pinning analysis [87, 93]. It was demonstrated that quasipinning of the GPCs in some cases would already follow from a quasipinning of the Pauli exclusion principle. In order to decide whether quasipinning as measured by D_{min} would have a relevance *beyond* the Pauli exclusion principle an additional measure was reviewed.

The Q -measure [94] compares the l_1 distances between the $\vec{\lambda}$ -vector and the polytope and Pauli simplex boundaries, respectively. It is a relative measure for the relevance of the GPCs. Large Q values correspond to a remarkably strong quasipinning which could not be expected from the approximate saturation of the Pauli exclusion principle.

Equipped with these tools, we have comprehensively examined the quasipinning effect by *analytical* means in the third chapter. We have introduced the model system of Harmonium, which consists of N harmonically interacting particles in an external harmonic trapping potential. In a first analytical treatment, Schilling [87] had found remarkably strong quasipinning $D_{min} \sim \kappa^8$ for the one-dimensional 3-Harmonium ground state. By systematically studying the influence of the particle number, the degree of spin polarisation and the role of dimensionality, we found that the competition between the fermionic antisymmetry and the energy minimisation gives rise to a sort of ‘microscopic Pauli pressure’.

For the ground state of fully spin-polarised one-dimensional N -Harmonium, the minimal distance was derived as $D_{min} \sim \kappa^{2N}$ for $N \geq 4$. The result shows that by adding particles to the system, the $\vec{\lambda}$ -vector is forced closer to the boundary of the polytope. Furthermore, we observed the emergence of a well-pronounced active space structure of NONs around the fermi level. The evaluation of the Q -measure confirmed the non-triviality of the quasipinning by two orders κ in the regime of weak and intermediate coupling strengths. For large κ , the quasipinning was found to become trivial.

In the next step, we have studied quasipinning of fully spin polarised N -Harmonium in quasi-one-dimensional systems and truly higher dimensional systems.

For $n = 2$ spatial dimensions, we found κ^4 quasipinning for $N = 3, 4, 5$ fermions, which grows stronger and becomes κ^6 quasipinning when $N = 6, 7$. We see that again

adding particles increases the quasipinning. However, by increasing the dimensionality quasipinning becomes weaker. This is a consequence of larger dimensions of the active spaces, which originate in the additional angular degrees of freedom. By evaluating the Q -measure, it was shown that quasipinning is only non-trivial for $N = 4$ particles.

For $n = 3$ spatial dimensions, the sizes of the active spaces made conclusive quasipinning analysis even more a challenge. For $N = 3, 4$ quasipinning of fourth order in κ was found, which for $N = 3$ might be even stronger. While trivial for $N = 4$, quasipinning for $N = 3$ becomes non-trivial by two orders in κ . Generally, increasing the dimensionality confirmed the notion of a ‘microscopic Pauli pressure’. This pressure, which still needs to be given a concise definition, illustrates for ground states the conflict between the energy minimisation and the fermionic antisymmetry.

In another approach to examine the influence of the dimensionality, we have considered dimensional crossovers by detuning trapping frequencies. This has qualitatively provided additional evidence for the existence and role of a microscopic Pauli pressure. The study of intermediate dimensions revealed that quasipinning is increased by narrowing the trapping potential and decreasing the interaction strength. In contrast to the absolute quasipinning, the Q -measure showed a much more complex behaviour. When the interaction strength is constant the detuning of the trapping frequencies causes multiple changes between different regimes with highly non-trivial and trivial quasipinning. This provided further evidence for the need to characterise the relevance of quasipinning of GPCs beyond the quasipinning of the Pauli exclusion principle. In particular, it would be interesting to apply the Q -measure to the findings on quasipinning in Refs. [7, 8, 9, 18].

By eventually considering spinful fermions, we observed that quasipinning strongly depends on the degree of spin polarisation. Using a variable external magnetic field, we discovered that for $N = 3, 4$ spinful fermions in one-dimensional Harmonium the minimal distance depends on the magnetisation M via $D_{min} \sim \kappa^{4+2|M|}$, i.e. quasipinning increases with the degree of spin-polarisation. Again, this provides evidence for the notion of the microscopic Pauli pressure since increasing the degree of spin-polarisation leads to reduced sizes of the active space structures.

Our findings on spinful fermions suggest the following idea for an experimental implementation of the quasipinning effect. Assume that a system of spinful fermions is prepared in a ground state which has NONs quasipinned to the polytope boundary. By applying an oscillating external magnetic field, the NONs will be perturbed.

Viewed in terms of the common one-particle picture and the Pauli exclusion principle, no restrictions would be imposed upon the evolution of the NONs. However, since the $\vec{\lambda}$ -vector is strongly quasipinned, only selected perturbations (perhaps by the polarisation of the magnetic field) will not violate the GPCs, which potentially gives rise to a *GPC-induced transparency*. Note that this is conceptually similar to the suppression of transitions in atoms which would cause a violation of the Pauli exclusion principle.

Future objectives of research on the GPCs comprise pinning analyses of further physical systems such as atoms. A major challenge in this is posed by the limited knowledge on settings of GPCs with one-particle Hilbert space dimensions larger than 11. Unfortunately, even truncated realistic physical systems (e.g. the Lithium atom) require at least 13 orbitals. GPCs might also be useful in effective energy functional methods such as DFT and RDMFT. We emphasise that all quasipinning analyses in this work have either been done analytically, or, if resorting to numerical diagonalisation of the 1-RDO, have been carried out with a well-controlled truncation error. The concept of a truncated pinning analyses, applied in this thesis, will allow for the conclusive study of GPCs in other systems as well.

In the fourth chapter of this thesis, we have studied the role of the exclusion principle in systems of hardcore bosons, where it only holds on a specific lattice one-particle basis. The constraint arises due to a large particle-particle interaction and can be implemented as a kinematical constraint by restricting the N -boson Hilbert space to the N -hardcore boson Hilbert space $\mathcal{H}_N^{(hcb)}$. This space is spanned by all N -permanents of N different lattice states, allowing only for single occupancies of every lattice site. Since hardcore bosons obey bosonic commutation relations, occupation numbers larger than one become possible, contrary to popular opinion. For the case of two hardcore bosons on three lattice sites, we have analytically determined the set of all compatible one-particle spectra. We found that this set is neither convex nor does it agree with the respective sets of bosons or fermions, providing first evidence for the hybrid character of hardcore bosons.

In the next step, we have considered an analogue of the Pauli exclusion principle for hardcore bosons. More specifically, we have proven a key theorem on the maximal occupation number λ_{max} of hardcore bosons.

$$\lambda_{max} = \frac{N}{d}(d - N + 1), \quad (5.1)$$

where N and d represent the number of particles and lattice sites. This occupation number is attained by any one-particle state which is mutually unbiased with respect

to the lattice basis. Furthermore, the theorem established that the maximising N -particle state is an equally weighted superposition of all permanents of the lattice basis. We have investigated the structural properties of this state and found that it resembles a bosonic superfluid state which has been projected to the hardcore Hilbert space. Furthermore, note that for $2N = d$ the thermodynamic limit of λ_{max} approaches $N/2$.

The theorem paved the way for the investigation of the one-body N -representability problem for hardcore bosons. In systems of hardcore bosons which only have 2-body interaction terms in the form of the hardcore interaction, the hardcore constraint can be implemented kinematically. Then, the energy functional solely depends on the 1-RDO. Therefore, a solution of the one-body N -representability problem would allow for an efficient description of this many-body system.

By using the Karush-Kuhn-Tucker-formalism, we derived general bounds on the traces of the m -th power of the 1-RDO, which provided necessary conditions for the N -representability of hardcore boson 1-RDOs. In some cases, these bounds have not yet been confirmed optimal and it remains an important objective of future research to verify conjecture 1. The computed bounds on $tr(\rho^m)$ give rise to outer approximations of the set of compatible one-particle spectra.

By applying a variational approach on parametrised expressions of $tr(\rho^m)$, we have developed a general algorithm, which in principle permits the computation of a complete set of necessary and sufficient conditions for hardcore boson N -representability of arbitrary settings (N, d) . A complete set of such conditions was calculated for $N = 3$ particles on $d = 4$ sites. The algorithm, though practically not feasible for larger settings, might be the starting point for an analysis of the complexity of the hardcore boson N -representability problem.

Next, we have studied one-particle entropy measures of hardcore bosons by again applying the Karush-Kuhn-Tucker-formalism. Our results for different entropy measures indicate that hardcore bosons exhibit a hybrid character. In systems with $d - N \leq 4$, the lower one-particle entropy resembles the fermionic case, whereas in the thermodynamic limit $d \rightarrow \infty$ the lower one-particle entropy approaches the bosonic case.

In the last section we have studied two physical systems whose ground states exhibit a maximally occupied orbital. In the first system, N hardcore bosons are placed in a star lattice with equal hopping rates between the ring sites and the central site. Although its ground state does not immediately saturate λ_{max} , a projective measurement on the central site can collapse it to a state maximising the occupation

number in the system of the ring sites. The second system we consider is known as the 1D quantum lattice gas. Despite comprising additional 2-body terms, it has a ground state at which λ_{max} is attained. Due to our earlier results on the structure of the respective 1-RDO, we find that the ground state of these two systems has long-range order correlations which do not vanish in the thermodynamic limit. Furthermore, both ground states show a *macroscopic* occupation of a single-particle state. The systems therefore provide a means for (fractional) Bose-Einstein condensation in strictly one-dimensional systems.

In a follow-up research project, both systems will also be the starting point for an investigation of the approximate saturation of the maximal hardcore boson occupation number. Depending on the parameters of the Hamiltonian, the 1D quantum lattice gas can be mapped to either a Heisenberg XXX chain or an XXZ chain. In future work, the exact diagonalisation of the XXZ chain can be used to derive an analytical expression for the 1-RDO with maximal occupation close to λ_{max} . By evaluating $\lambda_1(\delta)$ for some perturbation parameter δ , one can find a ‘quasipinning’ curve in the space of compatible one-particle spectra.

Appendix A

Examples of Generalised Pauli constraints

In the following, we present the GPCs of various settings (N, d) . For details on their derivation we refer to the cited literature.

For settings with $N = 2$ and arbitrary d , an application of the Schmidt decomposition establishes the conditions (cf. Ref. [84]):

$$\lambda_i = \lambda_{i+1}, \quad \text{for } i \text{ odd.} \quad (\text{A.1})$$

For the setting $(N, d) = (4, 8)$, there are 14 GPCs (see Ref. [1]):

$$\begin{aligned}
 D_1^{(4,8)}(\vec{\lambda}) &:= 0 - \lambda_5 + \lambda_6 + \lambda_7 + \lambda_8 \geq 0, \\
 D_2^{(4,8)}(\vec{\lambda}) &:= 0 - \lambda_1 + \lambda_2 + \lambda_7 + \lambda_8 \geq 0, \\
 D_3^{(4,8)}(\vec{\lambda}) &:= 0 - \lambda_1 + \lambda_3 + \lambda_6 + \lambda_8 \geq 0, \\
 D_4^{(4,8)}(\vec{\lambda}) &:= 0 - \lambda_1 + \lambda_4 + \lambda_6 + \lambda_7 \geq 0, \\
 D_5^{(4,8)}(\vec{\lambda}) &:= 0 - \lambda_1 + \lambda_4 + \lambda_5 + \lambda_8 \geq 0, \\
 D_6^{(4,8)}(\vec{\lambda}) &:= 0 - \lambda_3 + \lambda_4 + \lambda_7 + \lambda_8 \geq 0, \\
 D_7^{(4,8)}(\vec{\lambda}) &:= 0 - \lambda_2 + \lambda_4 + \lambda_6 + \lambda_8 \geq 0, \\
 D_8^{(4,8)}(\vec{\lambda}) &:= 2 - \lambda_2 - \lambda_3 - \lambda_5 + \lambda_8 \geq 0, \\
 D_9^{(4,8)}(\vec{\lambda}) &:= 2 - \lambda_1 - \lambda_3 - \lambda_6 + \lambda_8 \geq 0, \\
 D_{10}^{(4,8)}(\vec{\lambda}) &:= 2 - \lambda_1 - \lambda_2 - \lambda_7 + \lambda_8 \geq 0, \\
 D_{11}^{(4,8)}(\vec{\lambda}) &:= 2 - \lambda_1 - \lambda_2 - \lambda_3 + \lambda_4 \geq 0, \\
 D_{12}^{(4,8)}(\vec{\lambda}) &:= 2 - \lambda_1 - \lambda_4 - \lambda_5 + \lambda_8 \geq 0, \\
 D_{13}^{(4,8)}(\vec{\lambda}) &:= 2 - \lambda_1 - \lambda_2 - \lambda_5 + \lambda_6 \geq 0, \\
 D_{14}^{(4,8)}(\vec{\lambda}) &:= 2 - \lambda_1 - \lambda_3 - \lambda_5 + \lambda_7 \geq 0.
 \end{aligned} \quad (\text{A.2})$$

The following tables are taken from Ref. [94]. They display the GPCs of the settings $(3, 10)$, $(4, 10)$ and $(5, 10)$, which were originally computed by Klyachko and Altunbulak (see, e.g., Ref. [1]). Furthermore, the tables contain the minimal pairs (r, s) and the optimal prefactors c_j (cf. Sec. 2.5). By convention, the minimal pair $\{r, s\}$ is represented by $\{r, d + 1 - s\}$. If $\{\}$ contains only a single entry, then $\{t\}$ refers to $\{0, d + 1 - t\}$ if $t > N$ and $\{t, 0\}$, if $t \leq N$.

Setting $(N, d) = (3, 10)$

GPC	$\kappa^{(0)}$	$\kappa^{(1)}$	$\kappa^{(2)}$	$\kappa^{(3)}$	$\kappa^{(4)}$	$\kappa^{(5)}$	$\kappa^{(6)}$	$\kappa^{(7)}$	$\kappa^{(8)}$	$\kappa^{(9)}$	$\kappa^{(10)}$	$\{r, d + 1 - s\}$	c
1	1	-1	-1	1	-1	1	1	0	0	0	0	$\{1, 6\}$	1
2	1	-1	0	0	0	0	0	0	0	0	-1	$\{1, 10\}$	1/2
3	3	-2	0	0	0	-1	-1	-1	-1	0	-2		9/14
4	3	-2	-1	0	0	0	0	-1	-1	-1	-2	$\{3, 4\}$	1/2
5	3	-3	-2	2	1	0	0	0	0	-1	-2	$\{3, 4\}$	3/4
6	3	-3	1	0	0	0	0	-1	-2	2	-2		1
7	2	-1	0	-1	-1	0	-1	0	0	0	0	$\{7\}, \{1, 8\}$	1, 3/4
8	2	-1	-1	0	-1	0	0	-1	0	0	0	$\{1, 8\}$	3/4
9	2	-1	-1	0	0	-1	-1	0	0	0	0	$\{7\}, \{1, 8\}$	1, 3/4
10	2	0	-1	-1	-1	-1	0	0	0	0	0	$\{7\}$	1
11	3	-2	0	-1	-2	1	-1	0	0	0	-1	$\{1, 8\}$	5/4
12	3	-2	0	-1	-1	0	-2	1	0	0	-1	$\{7\}, \{1, 8\}$	2, 5/4
13	3	-1	0	-2	-2	0	-1	1	0	0	-1	$\{7\}$	2
14	3	-2	-1	0	0	0	-1	-1	-2	1	0	$\{3, 4\}$	2/5
15	3	-2	0	0	-1	-1	-2	1	-1	0	0		3/5
16	3	-2	0	0	-1	-1	-1	0	-2	1	0		3/5
17	3	-2	-1	0	0	-1	-2	1	0	0	-1	$\{7\}, \{1, 8\}$	2, 5/4
18	3	-1	-2	0	0	-2	-1	1	0	0	-1	$\{7\}$	2
19	3	0	-2	-1	-1	-2	0	1	0	0	-1	$\{7\}$	2
20	3	0	-1	-2	-2	-1	0	1	0	0	-1	$\{7\}$	2
21	3	0	-2	-1	-2	-1	1	0	0	0	-1	$\{1, 6\}$	1
22	3	-2	-1	0	-2	1	0	-1	0	0	-1	$\{1, 8\}$	5/4
23	3	-1	-2	0	-2	0	1	-1	0	0	-1	$\{1, 6\}$	1
24	3	-2	-1	0	-2	1	0	0	-1	-1	0	$\{1, 6\}$	1
25	3	-1	-2	0	-2	0	1	0	-1	-1	0	$\{1, 6\}$	1
26	3	-1	-2	0	-2	1	0	-1	0	-1	0	$\{3, 4\}$	1/3
27	3	-2	-2	1	-1	0	0	-1	0	0	-1	$\{1, 8\}$	5/4
28	3	-2	-2	1	-1	0	0	0	-1	-1	0	$\{1, 6\}$	1
29	3	0	-2	-1	-1	-2	1	0	0	-1	0	$\{1, 6\}$	1
30	3	0	-1	-2	-2	-1	1	0	0	-1	0	$\{1, 6\}$	1
31	3	-2	-2	1	0	-1	-1	0	0	0	-1	$\{1, 8\}$	5/4
32	3	-2	-2	1	0	0	-1	-1	-1	0	0	$\{3, 4\}$	2/5
33	2	-1	-2	1	0	-1	1	0	-1	1	0	$\{1, 6\}$	1
34	2	-1	0	-1	-2	1	1	0	-1	1	0	$\{1, 6\}$	1
35	2	0	-1	-1	-2	1	0	1	-1	1	0	$\{3, 4\}$	1/2
36	2	-1	-2	1	-1	1	0	0	-1	1	0	$\{3, 4\}$	1/3
37	1	0	-1	0	-1	0	1	0	0	0	0	$\{1, 6\}$	1/2
38	1	0	-1	0	0	-1	0	1	0	0	0	$\{7\}$	1
39	1	-1	0	0	-1	1	0	0	0	0	0	$\{1, 10\}$	1/2
40	1	-1	0	0	0	0	-1	1	0	0	0	$\{7\}, \{1, 10\}$	1, 1/2

GPC	$\kappa^{(0)}$	$\kappa^{(1)}$	$\kappa^{(2)}$	$\kappa^{(3)}$	$\kappa^{(4)}$	$\kappa^{(5)}$	$\kappa^{(6)}$	$\kappa^{(7)}$	$\kappa^{(8)}$	$\kappa^{(9)}$	$\kappa^{(10)}$	$\{r, d+1-s\}$	c
41	1	0	0	-1	-1	0	0	1	0	0	0	{7}	1
42	1	-1	-1	1	0	0	0	0	0	0	0	{1, 10}	1/2
43	1	-1	0	0	0	0	0	0	-1	1	0	{1, 10}	1/2
44	3	-2	0	0	0	-1	-1	-1	-2	1	-1		9/14
45	3	-2	-2	1	0	0	0	-1	-1	-1	-1	{3, 4}	1/2
46	3	-2	-1	0	-1	0	-1	0	-1	0	-1	{1, 10}	3/4
47	3	-1	-2	0	-1	-1	0	0	-1	0	-1	{1, 6}	1/2
48	3	-1	-1	-1	-2	0	0	0	-1	0	-1	{1, 6}	1/2
49	2	-1	-2	1	0	-1	1	0	0	0	-1	{1, 6}	1
50	2	-1	0	-1	-2	1	1	0	0	0	-1	{1, 6}	1
51	2	0	-1	-1	-2	1	0	1	0	0	-1	{3, 4}	1/2
52	3	-2	-3	2	0	1	0	-1	-2	2	1	{3, 4}	2/3
53	3	0	-1	-2	-3	2	1	0	-2	2	1	{3, 4}	3/4
54	3	-3	1	-1	-2	2	-2	2	1	0	0	{1, 8}	29/12
55	3	-2	1	-2	-3	2	-1	2	1	0	0	{1, 6}	2
56	3	-3	-2	2	1	0	0	-1	-2	2	1	{3, 4}	17/24
57	3	-3	1	0	0	-1	-2	2	-2	2	1		6/5
58	3	-3	-2	2	1	-1	-2	2	1	0	0	{1, 8}	29/12
59	3	-2	-3	2	1	-2	-1	2	1	0	0	{1, 6}	2
60	3	1	-3	-1	-2	-2	2	2	1	0	0	{1, 6}	2
61	3	1	-2	-2	-3	-1	2	2	1	0	0	{1, 6}	2
62	3	-2	-3	2	-2	2	1	0	-1	0	1	{3, 4}	2/3
63	3	-2	-3	2	-2	2	1	-1	0	1	0	{3, 4}	2/3
64	3	-3	-2	2	-2	2	1	-1	1	0	0	{1, 8}	29/12
65	3	-2	-2	1	-3	2	2	-1	1	0	0	{1, 6}	2
66	3	-2	-3	2	-2	1	2	-1	1	0	0	{1, 6}	2
67	3	-3	-2	2	-2	2	1	0	0	-1	1	{1, 6}	2
68	3	-2	-2	1	-3	2	2	0	0	-1	1	{1, 6}	2
69	3	-2	-3	2	-2	1	2	0	0	-1	1	{1, 6}	2
70	3	-4	-3	4	2	1	0	1	0	-1	-2	{3, 4}	7/6
71	3	-4	2	1	0	1	0	-1	-3	4	-2		3/2
72	4	-3	0	-1	0	-1	-2	1	0	-1	-2	{1, 10}	2
73	4	-3	0	-1	-2	1	0	-1	0	-1	-2	{1, 10}	2
74	4	-3	-2	1	0	-1	0	-1	0	-1	-2	{1, 10}	2
75	4	-1	-1	-2	-3	1	0	0	0	-1	-2	{3, 4}	8/15
76	4	-3	0	-1	0	-1	0	-1	-2	1	-2	{1, 10}	2
77	4	-2	-3	1	-1	0	0	-1	-2	1	0	{3, 4}	1/2
78	4	-1	-1	-2	-3	1	0	0	-2	1	0	{3, 4}	19/36
79	4	-3	0	-1	-2	1	-2	1	0	-1	0	{1, 10}	2
80	4	-3	0	-1	-2	1	0	-1	-2	1	0	{1, 10}	2
81	4	-2	0	-2	-3	1	-1	1	0	-1	0	{1, 6}	3/2
82	4	-3	-2	1	0	-1	0	-1	-2	1	0	{1, 10}	2
83	4	-3	0	-1	0	-1	-2	1	-2	1	0	{1, 10}	2
84	4	-3	-2	1	0	-1	-2	1	0	-1	0	{1, 10}	2
85	4	-2	-3	1	0	-2	-1	1	0	-1	0	{1, 6}	3/2
86	4	0	-3	-1	-2	-2	1	1	0	-1	0	{1, 6}	3/2
87	4	0	-2	-2	-3	-1	1	1	0	-1	0	{1, 6}	3/2
88	4	-2	-3	1	-2	1	0	-1	-1	0	0	{3, 4}	1/2
89	4	-3	-2	1	-2	1	0	-1	0	-1	0	{1, 10}	2
90	4	-2	-2	0	-3	1	1	-1	0	-1	0	{1, 6}	3/2
91	4	-2	-3	1	-2	0	1	-1	0	-1	0	{1, 6}	3/2
92	3	-4	2	1	0	1	0	-1	-2	3	-3		3/2
93	3	-4	-2	3	2	1	0	1	0	-1	-3	{3, 4}	7/6

Setting $(N, d) = (4, 10)$

GPC	$\kappa^{(0)}$	$\kappa^{(1)}$	$\kappa^{(2)}$	$\kappa^{(3)}$	$\kappa^{(4)}$	$\kappa^{(5)}$	$\kappa^{(6)}$	$\kappa^{(7)}$	$\kappa^{(8)}$	$\kappa^{(9)}$	$\kappa^{(10)}$	$\{r, d+1-s\}$	c
1	1	-1	0	0	0	0	0	0	0	0	0	{1}	1/2
2	3	-1	-1	-1	0	-1	0	0	0	-1	0	{2, 7}	1/2
3	3	-1	-1	-2	1	-2	2	1	2	0	0	{4, 5}	3/4
4	3	-1	-2	-1	1	-2	2	2	1	0	0	{2, 7}	2
5	3	-2	-1	-2	2	-1	2	1	1	0	0	{4, 5}	3/4
6	3	-1	-2	-2	2	-1	1	2	1	0	0	{2, 7}	2
7	4	-1	-2	-2	1	-3	3	2	2	0	0	{4, 5}	1
8	4	-2	-2	-3	3	-1	2	2	1	0	0	{4, 5}	1
9	5	-3	-1	-2	1	0	-1	1	0	-1	1	{2, 7}	7/4
10	5	-2	-1	-1	-1	-3	1	1	1	0	0	{2, 7}	5/4
11	5	-3	-1	0	-1	-2	1	1	0	-1	1	{2, 7}	7/4
12	5	-3	-1	-2	1	-1	1	0	0	-1	1	{4, 5}	5/8
13	5	-2	-3	-1	1	-1	1	0	0	-1	1	{2}	3/2
14	5	-2	-3	0	0	-1	1	-1	1	-1	1	{2}	3/2
15	5	-2	-3	-1	1	0	0	-1	1	-1	1	{2}	3/2
16	5	-3	0	-1	-1	-2	1	0	1	-1	1	{4, 5}	5/8
17	5	-2	-1	-3	1	-1	-1	1	1	0	0	{2, 7}	5/4
18	5	-2	-3	-1	1	-1	1	-1	1	0	0	{2}	3/2
19	2	-1	0	-1	0	-1	0	1	0	0	0	{7}	3/4
20	2	-1	0	0	-1	-1	0	0	1	0	0	{7}, {1, 8}	3/4, 2
21	2	-1	-1	0	0	0	0	0	0	-1	1	{2}	1/2
22	2	-1	-1	0	0	0	0	-1	1	0	0	{2}, {1, 8}	1/2, 2
23	2	0	-1	-1	0	-1	0	0	1	0	0	{7}	3/4
24	2	-1	0	-1	0	0	-1	0	1	0	0	{7}, {1, 8}	3/4, 2
25	2	-1	-1	0	0	-1	1	0	0	0	0	{2}	1/2
26	2	-1	-1	-1	1	0	0	0	0	0	0	{2}	1/2
27	4	-2	-1	-1	0	-1	0	0	-1	0	0	{2, 9}	1
28	4	-2	0	-1	-1	-1	-1	0	0	0	0	{7}, {1, 8}	1/2, 2
29	4	-2	-1	-1	0	0	-1	-1	0	0	0	{1, 8}, {2, 9}	2, 1
30	4	-2	-1	0	-1	-1	0	-1	0	0	0	{1, 8}, {2, 9}	2, 1
31	4	-1	-1	-1	-1	-2	0	0	0	0	0	{7}	1/2
32	4	-1	-1	-2	0	-1	-1	0	0	0	0	{7}	1/2
33	4	-1	-2	-1	0	-1	0	-1	0	0	0	{2, 9}	1
34	5	-2	-1	-1	-1	-2	0	0	0	-1	0	{2, 7}	3/4
35	5	-2	-2	-1	0	-1	0	-1	0	-1	0	{2}	3/4
36	5	-2	-1	-2	0	-1	-1	0	0	-1	0	{2, 7}	3/4
37	3	-2	-1	-1	1	-1	1	1	0	0	0	{2, 7}	5/4
38	3	-1	-1	-1	0	-2	1	1	1	0	0	{2, 7}	1
39	3	-1	-2	-1	1	-1	1	0	1	0	0	{2, 7}	5/4
40	3	-1	-1	-2	1	-1	0	1	1	0	0	{2, 7}	1
41	8	-2	-3	-4	1	-5	4	2	3	0	-1	{4, 5}	3/2
42	8	-2	-3	-4	1	-5	4	3	2	-1	0	{4, 5}	3/2

GPC	$\kappa^{(0)}$	$\kappa^{(1)}$	$\kappa^{(2)}$	$\kappa^{(3)}$	$\kappa^{(4)}$	$\kappa^{(5)}$	$\kappa^{(6)}$	$\kappa^{(7)}$	$\kappa^{(8)}$	$\kappa^{(9)}$	$\kappa^{(10)}$	$\{r, d+1-s\}$	c
43	8	-3	-4	-5	4	-2	2	3	1	0	-1	{4, 5}	3/2
44	8	-4	-3	-5	4	-2	3	2	1	0	-1	{4, 5}	3/2
45	8	-3	-4	-5	4	-2	3	2	1	-1	0	{4, 5}	3/2
46	8	-2	-4	-3	1	-5	4	3	2	0	-1	{4, 5}	3/2
47	8	-3	-1	-2	-2	-3	0	0	-1	-2	0	{4, 5}	1/2
48	6	-2	-1	-3	0	-1	-2	1	0	0	-1	{7}	3/2
49	6	-1	-2	-3	0	-2	-1	1	0	0	-1	{7}	3/2
50	6	-3	-2	0	0	-1	-1	-2	1	-1	0		6/5
51	6	-3	-2	0	0	-1	-1	-1	0	-2	1		6/5
52	6	-3	-2	-1	0	0	0	-1	-1	-2	1	{4, 5}	3/4
53	6	-3	-1	-2	0	-2	0	1	0	-1	-1	{2, 7}	3/2
54	6	-3	-1	-2	0	-2	1	0	-1	0	-1	{4, 5}	7/12
55	6	-3	0	-1	-2	-2	-1	1	0	0	-1	{7}	3/2
56	6	-3	0	-2	-1	-1	-2	1	0	0	-1	{7}	3/2
57	6	-3	-2	-1	0	-2	1	0	0	-1	-1	{2, 7}	5/4
58	6	-3	-2	-2	1	0	0	-1	-1	-1	0	{4, 5}	3/4
59	6	-2	-1	-1	-2	-3	0	1	0	0	-1	{7}	3/2
60	6	-2	-1	-1	-2	-3	1	0	0	-1	0	{4, 5}	7/12
61	6	-3	-2	-2	1	-1	0	0	0	-1	-1	{2, 7}	5/4
62	6	-1	-2	-2	-1	-3	0	1	0	0	-1	{7}	3/2
63	6	-2	-1	-2	-1	-3	1	0	0	0	-1	{4, 5}	11/20
64	6	-1	-2	-2	-1	-3	1	0	0	-1	0	{4, 5}	7/12
65	8	-2	-2	-3	-1	-5	2	2	1	0	0	{4, 5}	1
66	8	-3	-1	-2	-2	-5	2	2	1	0	0	{4, 5}	1
67	8	-5	0	-1	-2	-3	2	1	0	-2	2	{4, 5}	1
68	8	-5	-2	-3	2	0	1	0	-1	-2	2	{4, 5}	5/4
69	8	-5	-3	1	0	0	-1	-2	2	-2	2		12/5
70	8	-5	-3	-2	2	1	0	0	-1	-2	2	{4, 5}	5/4
71	8	-5	-2	-3	2	-2	2	1	0	-1	0	{4, 5}	7/6
72	8	-5	-2	-2	1	-3	2	2	0	0	-1	{2, 7}	11/4
73	8	-5	-2	-3	2	-2	1	2	0	0	-1	{2, 7}	11/4
74	8	-5	-3	-2	2	-2	2	1	0	0	-1	{2, 7}	5/2
75	4	-2	-3	-1	2	-1	2	0	1	1	0	{2}	2
76	4	-2	-3	0	1	-1	2	-1	2	1	0	{2}	2
77	4	-1	-3	-1	1	-2	2	0	2	1	0	{2, 7}	2
78	4	-2	0	-3	1	-1	-1	2	2	1	0	{7}	3/2
79	4	-2	-1	-3	2	0	-1	1	2	1	0	{2, 7}	7/4
80	4	-1	-1	-3	1	-2	0	2	2	1	0	{7}	3/2
81	4	-1	-2	-3	2	-1	0	1	2	1	0	{2, 7}	7/4
82	4	-2	-3	-1	2	0	1	-1	2	1	0	{2}	2
83	4	-1	-3	-2	2	-1	1	0	2	1	0	{2, 7}	2
84	4	-3	-1	1	-1	-2	2	0	2	1	0	{2, 7}	2
85	4	-3	-1	-2	2	1	-1	0	2	1	0	{2, 7}	2
86	4	-3	-2	1	0	-1	2	-1	2	1	0	{2}	2

GPC	$\kappa^{(0)}$	$\kappa^{(1)}$	$\kappa^{(2)}$	$\kappa^{(3)}$	$\kappa^{(4)}$	$\kappa^{(5)}$	$\kappa^{(6)}$	$\kappa^{(7)}$	$\kappa^{(8)}$	$\kappa^{(9)}$	$\kappa^{(10)}$	$\{r, d+1-s\}$	c
87	4	-3	-2	-1	2	1	0	-1	2	1	0	{2}	2
88	4	-3	1	-1	-1	-2	0	2	2	1	0	{7}	3/2
89	4	-3	1	-2	0	-1	-1	2	2	1	0	{7}	3/2
90	4	-2	-1	-3	2	-1	0	2	1	1	0	{2, 7}	7/4
91	4	-3	-1	-2	2	-1	1	2	0	1	0	{2, 7}	2
92	4	-3	-1	-1	1	-2	2	2	0	1	0	{2, 7}	2
93	4	-3	-2	-1	2	-1	2	1	0	1	0	{2}	2
94	4	-2	-1	0	-1	-3	2	1	2	1	0	{2, 7}	7/4
95	4	-1	-2	-1	0	-3	2	1	2	1	0	{2, 7}	7/4
96	4	-2	0	-1	-1	-3	1	2	2	1	0	{7}	3/2
97	4	-1	-1	-2	0	-3	1	2	2	1	0	{7}	3/2
98	4	-2	-1	-1	0	-3	2	2	1	1	0	{2, 7}	7/4
99	4	-3	-2	1	0	-1	2	1	0	-1	2	{2}	2
100	4	-1	-2	-3	2	-1	1	0	2	0	1	{4, 5}	3/4
101	4	-2	-3	-1	2	1	0	0	1	-1	2	{2}	2
102	4	-2	-3	-1	2	1	0	-1	2	0	1	{2}	2
103	4	-2	-3	1	0	-1	2	-1	2	0	1	{2}	2
104	4	-2	-3	1	0	0	1	-1	2	-1	2	{2}	2
105	4	-2	-3	1	0	-1	2	0	1	-1	2	{2}	2
106	4	-2	-3	-1	2	0	1	1	0	-1	2	{2}	2
107	4	-2	-3	0	1	-1	2	1	0	-1	2	{2}	2
108	4	-2	-3	0	1	1	0	-1	2	-1	2	{2}	2
109	4	-3	-2	1	0	1	0	-1	2	-1	2	{2}	2
110	4	-3	-2	-1	2	1	0	1	0	-1	2	{2}	2
111	4	-2	-3	-1	2	-1	2	1	0	0	1	{2}	2
112	4	-2	-1	0	-1	-3	2	2	1	0	1	{2, 7}	2
113	4	-3	-1	-2	2	-1	2	1	0	0	1	{4, 5}	5/6
114	4	-2	0	-1	-1	-3	2	1	2	0	1	{4, 5}	3/4
115	4	-2	-1	-3	2	0	-1	2	1	0	1	{2, 7}	2
116	4	-3	0	0	-1	-2	2	1	1	-1	2	{4, 5}	3/4
117	4	-3	-1	-2	2	0	1	1	0	-1	2	{4, 5}	5/6
118	4	-1	-2	-1	0	-3	2	2	1	0	1	{2, 7}	2
119	4	-1	-1	-2	0	-3	2	1	2	0	1	{4, 5}	3/4
120	4	-1	-2	-3	2	-1	0	2	1	0	1	{2, 7}	2
121	7	-2	-3	-4	2	-2	0	2	1	0	-1	{2, 7}	5/2
122	7	-2	-2	-3	0	-4	2	1	2	0	-1	{4, 5}	1
123	7	-2	-2	-3	0	-4	2	2	1	-1	0	{4, 5}	1
124	7	-4	-2	-3	2	-2	2	1	0	0	-1	{4, 5}	25/24
125	7	-2	-3	-2	0	-4	2	2	1	0	-1	{2, 7}	5/2

Setting $(N, d) = (5, 10)$

GPC	$\kappa^{(0)}$	$\kappa^{(1)}$	$\kappa^{(2)}$	$\kappa^{(3)}$	$\kappa^{(4)}$	$\kappa^{(5)}$	$\kappa^{(6)}$	$\kappa^{(7)}$	$\kappa^{(8)}$	$\kappa^{(9)}$	$\kappa^{(10)}$	$\{r, d+1-s\}$	c
1	1	-1	0	0	0	0	0	0	0	0	0	{1}	1/2
2	4	0	-1	-1	-1	-1	-1	-1	0	0	0	{1, 8}	1/2
3	3	-1	-1	-1	0	0	0	0	0	0	-1	{3, 10}	1/2
4	2	0	-1	-1	-1	1	0	0	0	1	1	{3, 8}	5/6
5	2	-1	-1	0	0	0	-1	1	1	1	0	{3, 8}	5/6
6	2	0	-1	-1	0	0	-1	1	0	1	1	{3, 8}	5/6
7	2	-1	-1	-1	0	1	0	1	0	1	0	{3, 10}	3/4
8	2	-1	-1	0	-1	1	0	0	1	1	0	{3, 8}	5/6
9	2	0	-1	0	-1	0	-1	0	1	1	1	{1, 8}	3/4
10	6	-2	-2	-3	1	0	1	0	-1	2	-1	{3, 10}	2
11	6	-2	-2	-3	-1	2	1	0	1	0	-1	{3, 10}	2
12	6	0	-1	-2	-3	0	-1	-2	2	1	1	{1, 8}	2
13	6	-2	-2	-3	1	0	-1	2	1	0	-1	{3, 10}	2
14	6	0	-3	0	-1	-2	-1	-2	2	1	1	{1, 8}	2
15	6	0	-3	0	-1	-1	-2	-2	1	2	1		17/9
16	6	0	-1	-2	-1	-2	-3	0	2	1	1	{1, 8}	2
17	6	-2	-3	-2	-1	2	1	1	0	0	-1	{5, 6}	1
18	6	0	-1	-1	-2	-2	-3	0	1	2	1	{5, 6}	1
19	6	-2	-3	-2	1	1	0	0	-1	2	-1		17/9
20	7	-1	-2	-1	-3	0	-3	0	2	2	1	{1, 8}	7/4
21	7	-1	-3	0	-3	0	-2	-1	2	2	1	{1, 8}	7/4
22	7	-2	-3	0	-3	1	-1	-1	2	2	0	{3, 8}	11/6
23	7	-2	-3	-1	-3	2	-1	0	2	1	0	{3, 8}	2
24	7	-1	-3	0	-2	-1	-3	0	2	2	1	{1, 8}	7/4
25	7	-2	-3	-3	-1	2	0	1	-1	2	0	{3, 10}	7/4
26	7	-2	-3	-3	-1	2	-1	2	0	1	0	{3, 10}	7/4
27	7	-2	-3	-1	-3	2	0	-1	1	2	0	{3, 8}	2
28	7	-1	-2	-3	0	-1	-3	2	0	1	2	{3, 8}	13/6
29	7	-1	-3	-2	0	-1	-3	2	0	2	1	{3, 8}	2
30	7	-1	-2	-3	-1	0	-3	2	0	2	1	{3, 8}	2
31	7	-2	-3	0	-1	-1	-3	1	2	2	0	{3, 8}	11/6
32	7	-2	-3	-1	-1	0	-3	2	2	1	0	{3, 8}	2
33	7	-2	-3	-3	0	1	-1	2	-1	2	0	{3, 10}	7/4
34	7	-1	-3	-3	0	0	-2	2	-1	2	1	{3, 8}	11/6
35	7	-3	-2	-1	-3	2	0	-1	2	1	0	{3, 8}	13/6
36	7	-1	-3	-3	-2	2	0	0	-1	2	1	{3, 8}	11/6
37	7	-1	-2	-3	-3	2	-1	0	0	2	1	{3, 8}	2
38	7	-2	-3	-1	0	-1	-3	2	1	2	0	{3, 8}	2
39	7	-1	-3	-2	-3	2	0	-1	0	2	1	{3, 8}	2
40	7	-3	-2	-3	1	0	-1	2	-1	2	0	{3, 10}	2
41	7	-1	-3	0	-3	0	-1	-2	2	1	2	{1, 8}	2
42	7	-3	-2	0	-1	-1	-3	2	1	2	0	{5, 6}	19/20

GPC	$\kappa^{(0)}$	$\kappa^{(1)}$	$\kappa^{(2)}$	$\kappa^{(3)}$	$\kappa^{(4)}$	$\kappa^{(5)}$	$\kappa^{(6)}$	$\kappa^{(7)}$	$\kappa^{(8)}$	$\kappa^{(9)}$	$\kappa^{(10)}$	$\{r, d+1-s\}$	c
43	7	-1	-3	-2	-3	2	0	0	-1	1	2	{5, 6}	19/20
44	7	-1	-2	-3	-3	2	0	-1	0	1	2	{3, 8}	13/6
45	7	-3	-2	-1	0	-1	-3	2	2	1	0	{3, 8}	13/6
46	7	-3	-1	-2	-3	2	-1	1	0	2	0	{5, 6}	19/20
47	7	-1	-3	-1	-2	0	-3	2	1	0	2	{5, 6}	19/20
48	7	-3	-1	-2	-3	2	-1	0	2	1	0	{3, 8}	2
49	7	-1	-2	-3	-1	0	-3	2	1	0	2	{3, 8}	2
50	7	-1	-3	-2	-3	2	-1	1	0	0	2	{5, 6}	19/20
51	7	-3	-1	-1	-2	0	-3	2	1	2	0	{5, 6}	19/20
52	7	-3	-1	-2	-1	0	-3	2	2	1	0	{3, 8}	2
53	7	-1	-2	-3	-3	2	-1	0	1	0	2	{3, 8}	2
54	7	-3	-2	-3	-1	2	1	0	-1	2	0	{3, 10}	2
55	7	-1	-3	0	-1	-2	-3	0	2	1	2	{1, 8}	2
56	7	-1	-1	-2	-3	0	-3	0	2	1	2	{1, 8}	2
57	7	-3	-2	-3	-1	2	-1	2	1	0	0	{3, 10}	2
58	7	-1	-1	-2	-3	0	-3	1	0	2	2	{5, 6}	31/30
59	7	-3	-3	-1	-2	2	-1	2	1	0	0	{5, 6}	31/30
60	9	-3	-4	-5	-1	4	3	2	1	0	-2	{5, 6}	2
61	9	-3	-4	-5	3	2	1	0	-1	4	-2		11/3
62	9	1	-5	0	-1	-2	-3	-4	4	3	2		11/3
63	9	1	-1	-2	-3	-4	-5	0	4	3	2	{5, 6}	2
64	4	-1	-2	0	-2	1	0	-1	2	1	0	{3, 8}	7/4
65	4	0	-1	-2	0	-1	-2	1	0	2	1	{3, 8}	7/4
66	4	-2	-2	-1	1	1	0	0	-1	2	0		3/2
67	4	0	-1	-2	-2	1	0	0	-1	1	2	{5, 6}	7/10
68	4	-2	0	-1	-1	0	-2	2	1	1	0	{5, 6}	13/20
69	4	0	-1	-2	-2	1	0	-1	0	2	1	{3, 8}	7/4
70	4	0	-2	-1	-2	1	0	0	-1	2	1	{5, 6}	7/10
71	4	-2	-1	0	0	-1	-2	2	1	1	0	{5, 6}	11/16
72	4	-2	-2	-1	-1	2	1	1	0	0	0	{5, 6}	4/5
73	4	0	-1	-1	-2	0	-2	1	0	2	1	{5, 6}	7/10
74	4	-1	-2	0	-1	0	-2	2	1	1	0	{5, 6}	13/20
75	4	-1	-2	0	0	-1	-2	1	2	1	0	{3, 8}	7/4
76	4	0	-2	0	-1	-1	-2	0	2	1	1	{1, 8}	3/2
77	4	0	-1	-1	-2	0	-2	0	2	1	1	{1, 8}	3/2
78	4	0	-2	0	-2	0	-1	-1	2	1	1	{1, 8}	3/2
79	2	0	-2	1	0	0	-1	-1	1	2	2		3/2
80	2	0	-1	-2	1	0	-1	2	0	2	1	{3, 8}	7/4
81	2	-1	-2	0	-1	2	1	0	2	1	0	{3, 8}	7/4
82	2	-2	-1	1	0	0	-1	2	2	1	0	{5, 6}	7/10
83	2	0	-1	-1	-2	2	0	1	1	0	2	{5, 6}	13/20
84	2	-1	-2	0	1	0	-1	2	2	1	0	{3, 8}	7/4
85	2	-1	-2	1	0	0	-1	2	1	2	0	{5, 6}	7/10
86	2	0	-1	-1	-2	2	1	0	0	1	2	{5, 6}	11/16

GPC	$\kappa^{(0)}$	$\kappa^{(1)}$	$\kappa^{(2)}$	$\kappa^{(3)}$	$\kappa^{(4)}$	$\kappa^{(5)}$	$\kappa^{(6)}$	$\kappa^{(7)}$	$\kappa^{(8)}$	$\kappa^{(9)}$	$\kappa^{(10)}$	$\{r, d+1-s\}$	c
87	2	-1	-2	0	-1	2	0	2	1	1	0	$\{5, 6\}$	7/10
88	2	0	-1	-1	-2	2	0	1	0	2	1	$\{5, 6\}$	13/20
89	2	0	-1	-2	-1	2	1	0	0	2	1	$\{3, 8\}$	7/4
90	2	-1	-1	-2	1	1	0	2	0	2	0	$\{3, 10\}$	3/2
91	2	0	0	0	-1	-1	-2	1	1	2	2	$\{5, 6\}$	4/5
92	2	-1	-1	-2	0	2	0	2	1	1	0	$\{3, 10\}$	3/2
93	2	-1	-1	-2	0	2	1	1	0	2	0	$\{3, 10\}$	3/2
94	3	0	-1	-1	-1	0	-1	0	0	0	1	$\{3, 8\}$	2/3
95	3	-1	0	-1	-1	0	-1	0	0	1	0	$\{1, 8\}$	1
96	3	-1	-1	0	0	-1	-1	0	0	1	0	$\{1, 8\}, \{2, 9\}$	1, 2
97	3	-1	-1	-1	0	0	-1	1	0	0	0	$\{3, 10\}$	1/2
98	3	-1	-1	0	-1	0	0	-1	0	1	0	$\{1, 8\}, \{2, 9\}$	1, 2
99	3	-1	-1	0	-1	0	-1	0	1	0	0	$\{1, 8\}$	1
100	3	-1	-1	-1	-1	1	0	0	0	0	0	$\{3, 10\}$	1/2
101	3	-1	-1	-1	0	0	0	0	-1	1	0	$\{2, 9\}, \{3, 10\}$	2, 1/2
102	5	-1	-2	-1	-1	0	-1	0	0	-1	0	$\{3, 10\}$	1
103	5	-2	-1	-1	-1	0	-1	0	0	0	-1	$\{3, 8\}$	2/3
104	5	-1	-2	-1	-1	0	0	-1	-1	0	0	$\{2, 9\}, \{3, 10\}$	2, 1
105	5	-1	-2	-1	0	-1	-1	0	-1	0	0	$\{2, 9\}, \{3, 10\}$	2, 1
106	5	-1	-1	-1	-1	-1	-2	0	0	0	0	$\{1, 8\}$	1/2
107	5	-1	-1	-2	-1	0	-1	0	-1	0	0	$\{3, 10\}$	1
108	5	-1	-2	0	-1	-1	-1	-1	0	0	0	$\{1, 8\}, \{2, 9\}$	1/2, 2
109	5	-1	-1	-1	-2	0	-1	-1	0	0	0	$\{1, 8\}$	1/2
110	6	0	-2	-1	-2	-1	-3	0	2	2	1	$\{1, 8\}$	7/4
111	6	0	-3	0	-2	-1	-2	-1	2	2	1	$\{1, 8\}$	7/4
112	6	0	-2	-1	-3	0	-2	-1	2	2	1	$\{1, 8\}$	7/4
113	6	0	-3	0	-1	-2	-1	-2	1	2	2	$\{1, 8\}$	2
114	6	0	-1	-2	-2	-1	-3	1	0	2	2	$\{5, 6\}$	31/30
115	6	0	-2	-1	-1	-2	-3	0	2	1	2	$\{1, 8\}$	2
116	6	0	-2	-1	-3	0	-1	-2	2	1	2	$\{1, 8\}$	2
117	6	0	-1	-2	-1	-2	-3	0	1	2	2	$\{1, 8\}$	2
118	6	0	-1	-2	-3	0	-1	-2	1	2	2	$\{1, 8\}$	2
119	6	0	-1	-2	-3	0	-2	-1	2	1	2	$\{1, 8\}$	2
120	6	0	-3	0	-2	-1	-1	-2	2	1	2	$\{1, 8\}$	2
121	6	0	-3	0	-1	-2	-2	-1	2	1	2	$\{1, 8\}$	2
122	6	0	-2	-2	-3	1	0	-1	-1	2	2	$\{5, 6\}$	19/20
123	6	0	-1	-2	-2	-1	-3	0	2	1	2	$\{1, 8\}$	2
124	6	-2	-2	0	-1	-1	-3	2	2	1	0	$\{5, 6\}$	17/20
125	7	-3	-2	-3	1	0	0	1	-1	2	-1	$\{3, 10\}$	2
126	7	-3	-2	-3	0	1	1	0	-1	2	-1	$\{3, 10\}$	2
127	7	-3	-3	-2	1	0	1	0	-1	2	-1	$\{3, 10\}$	2
128	7	-3	-3	-1	-2	2	0	1	1	0	-1	$\{5, 6\}$	31/30
129	7	-3	-2	-3	-1	2	1	0	0	1	-1	$\{3, 10\}$	2
130	7	-3	-2	-3	1	0	-1	2	0	1	-1	$\{3, 10\}$	2

GPC	$\kappa^{(0)}$	$\kappa^{(1)}$	$\kappa^{(2)}$	$\kappa^{(3)}$	$\kappa^{(4)}$	$\kappa^{(5)}$	$\kappa^{(6)}$	$\kappa^{(7)}$	$\kappa^{(8)}$	$\kappa^{(9)}$	$\kappa^{(10)}$	$\{r, d+1-s\}$	c
131	7	-3	-3	-2	-1	2	1	0	1	0	-1	$\{3, 10\}$	2
132	7	-3	-3	-2	1	0	-1	2	1	0	-1	$\{3, 10\}$	2
133	7	-3	-2	-3	0	1	-1	2	1	0	-1	$\{3, 10\}$	2
134	7	-3	-3	0	0	-1	-2	2	1	1	-1	$\{5, 6\}$	19/20
135	7	-3	-2	-3	-1	2	0	1	1	0	-1	$\{3, 10\}$	2
136	7	-2	-3	-3	0	1	-1	2	0	1	-1	$\{3, 10\}$	7/4
137	7	-2	-3	-3	-1	2	0	1	0	1	-1	$\{3, 10\}$	7/4
138	7	-2	-3	-3	0	1	0	1	-1	2	-1	$\{3, 10\}$	7/4
139	7	-1	-2	-3	-3	2	0	0	-1	1	1	$\{5, 6\}$	17/20
140	12	-2	-3	-4	-5	2	0	-1	-2	1	0	$\{5, 6\}$	9/8
141	12	-4	-5	0	-1	-2	-3	2	1	0	-2	$\{5, 6\}$	6/5
142	12	-4	-5	-3	1	0	0	-1	-2	2	-2		8/3
143	12	-4	-5	-3	-2	2	1	0	0	-1	-2	$\{5, 6\}$	43/30
144	12	-4	-5	-2	-3	2	0	1	0	-1	-2	$\{5, 6\}$	7/5
145	8	-2	-3	0	-1	-2	-4	3	2	1	0	$\{5, 6\}$	9/8
146	8	0	-2	-3	-4	1	0	-1	-2	3	2	$\{5, 6\}$	6/5
147	8	0	-1	-2	-3	-2	-4	1	0	3	2	$\{5, 6\}$	7/5
148	8	0	-4	0	-1	-2	-2	-3	1	3	2		8/3
149	8	0	-1	-2	-2	-3	-4	0	1	3	2	$\{5, 6\}$	43/30
150	4	-2	-2	-1	0	1	1	1	0	0	-1	$\{5, 6\}$	4/5
151	4	-2	-2	-1	1	1	0	0	0	1	-1		13/9
152	6	0	-2	-1	-1	-1	-2	-2	0	1	1		13/9
153	6	0	-1	-1	-2	-2	-2	-1	0	1	1	$\{5, 6\}$	4/5
154	15	-1	-7	0	-2	-3	-4	-5	3	2	1		11/3
155	15	-1	-2	-3	-4	-5	-7	0	3	2	1	$\{5, 6\}$	2
156	9	-3	-4	-5	3	2	1	0	-2	5	-1		11/3
157	9	-3	-4	-5	-2	5	3	2	1	0	-1	$\{5, 6\}$	2
158	8	0	-1	-2	-2	-3	-4	0	2	2	1	$\{5, 6\}$	4/3
159	8	0	-4	0	-1	-2	-2	-3	2	2	1		22/9
160	11	-3	-4	-4	-2	2	1	0	0	-1	-2	$\{5, 6\}$	4/3
161	11	-3	-4	-4	1	0	0	-1	-2	2	-2		22/9

Appendix B

Ground state and 1-RDO of Harmonium

B.1 Derivation of the Harmonium ground state

In this appendix, the ground state(s) of the Harmonium Hamiltonian (3.1) will be derived, providing a neat proof of Thm. 3.

First, let us consider the Hamiltonian (3.1) to act as an operator on the Hilbert space $\mathcal{H}_N \equiv L_2[\mathbb{R}^n]^{\otimes N}$ of N *distinguishable* particles. In that case, the diagonalisation can straightforwardly be achieved by a transformation to the center-of-mass ($y_1^{(\alpha)}$) and ‘relative’ coordinates ($y_k^{(\alpha)}, k = 2, \dots, N$) for all n spatial dimensions $\alpha = 1, \dots, n$ (see, e.g., Ref. [83] for the case $n = 1$), which decouples the harmonic oscillators. The eigenstates read

$$\begin{aligned} \Phi_{\boldsymbol{\nu}}^{(\boldsymbol{\omega}, \mathbf{K})}(\vec{x}_1, \dots, \vec{x}_N) &= \mathcal{N}_{\boldsymbol{\nu}}^{(\boldsymbol{\omega}, \mathbf{K})} \cdot \left[\prod_{\alpha=1}^n \varphi_{\nu_1^{(\alpha)}}^{(l^{(\alpha)})}(y_1^{(\alpha)}(x_1^{(\alpha)}, \dots, x_N^{(\alpha)})) \right] \\ &\times \left[\prod_{\alpha=1}^n \prod_{k=2}^N \varphi_{\nu_k^{(\alpha)}}^{(\tilde{l}^{(\alpha)})}(y_k^{(\alpha)}(x_1^{(\alpha)}, \dots, x_N^{(\alpha)})) \right], \end{aligned} \quad (\text{B.1})$$

where $\boldsymbol{\nu} \equiv (\nu_k^{(\alpha)})$, $\nu_k^{(\alpha)} \in \mathbb{N}_0$, $k = 1, \dots, N$, $\alpha = 1, \dots, n$, $\boldsymbol{\omega} \equiv (\omega^\alpha)$, $\mathbf{K} \equiv (K^{(\alpha)})$ and $\mathcal{N}_{\boldsymbol{\nu}}^{(\boldsymbol{\omega}, \mathbf{K})}$ denotes a normalisation constant. The natural lengths $l^{(\alpha)} = \sqrt{\frac{\hbar}{m\omega^{(\alpha)}}}$ and $\tilde{l}^{(\alpha)} = \sqrt{\frac{\hbar}{m\tilde{\omega}^{(\alpha)}}}$ are associated with the center-of-mass and relative motion in the α direction, respectively. The related characteristic frequencies are given by $(\omega^{(\alpha)})$ and

$$\tilde{\omega}^{(\alpha)} \equiv \sqrt{(\omega^{(\alpha)})^2 + \frac{NK^{(\alpha)}}{m}}. \quad (\text{B.2})$$

The center-of-mass coordinates $y_1^{(\alpha)}(x_1^{(\alpha)}, \dots, x_N^{(\alpha)})$ are (linear) symmetric functions of the physical coordinates $x_1^{(\alpha)}, \dots, x_N^{(\alpha)}$. By contrast, no unambiguous definition of

the relative coordinates exists which, however, is not required for our derivation. We remark that $\Phi_{\boldsymbol{\nu}}^{(\boldsymbol{\omega}, \mathbf{K})}$ explicitly depends on the couplings $(\boldsymbol{\omega}, \mathbf{K})$ which will become important below.

When omitting a constant energy off-set, the energy eigenvalues of the eigenstates (B.1) read

$$E_{\boldsymbol{\nu}}^{(\boldsymbol{\omega}, \mathbf{K})} = \sum_{\alpha=1}^n \hbar \omega^{(\alpha)} \nu_1^{(\alpha)} + \sum_{\alpha=1}^n \hbar \tilde{\omega}^{(\alpha)} \sum_{k=2}^N \nu_k^{(\alpha)}. \quad (\text{B.3})$$

Next, consider the space of coupling parameters

$$\Omega \equiv \{(\boldsymbol{\omega}, \mathbf{K}) \in (\mathbb{R}^+)^n \times \mathbb{R}^n \mid \forall \alpha : NK^{(\alpha)} > -m(\omega^{(\alpha)})^2\}. \quad (\text{B.4})$$

Since most energies $E_{\boldsymbol{\nu}}^{(\boldsymbol{\omega}, \mathbf{K})}$ are degenerate on Ω , it proves useful to identify the respective elements $\boldsymbol{\nu}$ and define corresponding equivalence classes $[\boldsymbol{\nu}]$. Based on these equivalence classes, one can describe the associated degenerate and finite dimensional eigenspaces

$$\mathcal{H}_{[\boldsymbol{\nu}]}^{(\boldsymbol{\omega}, \mathbf{K})} \equiv \text{span} \left(\left\{ \Phi_{\boldsymbol{\nu}'}^{(\boldsymbol{\omega}, \mathbf{K})} \mid \boldsymbol{\nu}' \in [\boldsymbol{\nu}] \right\} \right), \quad (\text{B.5})$$

which analytically depend on the coupling parameters $(\boldsymbol{\omega}, \mathbf{K}) \in \Omega$.

The fermionic ground state of the Hamiltonian (3.1) at a fixed set of coupling parameters $(\boldsymbol{\omega}, \mathbf{K}) \in \Omega$ may be derived by considering the projector $\mathcal{A}_N$ of the N -particle Hilbert space onto the N -fermion Hilbert space (cf. Eq. (2.5)). Specifically, the fermionic ground state is given by an element of $\mathcal{A}_N \mathcal{H}_{[\boldsymbol{\nu}]}^{(\boldsymbol{\omega}, \mathbf{K})}$ with $\boldsymbol{\nu}$ the minimiser of (B.3) under the constraint $\mathcal{A}_N \mathcal{H}_{[\boldsymbol{\nu}]}^{(\boldsymbol{\omega}, \mathbf{K})} \neq 0$.

Generally, the explicit form of the relative coordinates $y_i^{(\alpha)}$ makes it difficult to arrive at an elementary expression for $\mathcal{A}_N$ -projected states. Fortunately, the fermionic ground state can be given a concise form:

1. Since the center-of-mass coordinate in (B.1) is symmetric in the physical coordinates, the antisymmetrisation operator commutes with the respective functions $\varphi_{\nu_1^{(\alpha)}}$. Therefore, the lowest energy is achieved for $\vec{\nu}_1 = 0$ and the fermionic ground state lies in the eigenspace of zero center-of-mass excitation.
2. In the next step, one constructs a map of the coupling parameter points $(\boldsymbol{\omega}, \mathbf{K}) \in \Omega$ with finite particle-particle interaction strength to the points with zero interaction $(\boldsymbol{\omega}', \mathbf{K}') \equiv (\boldsymbol{\omega}', \mathbf{0})$ by requiring

$$\omega'^{(\alpha)} \equiv \sqrt{(\omega^{(\alpha)})^2 + \frac{NK^{(\alpha)}}{m}}, \quad \alpha = 1, \dots, n. \quad (\text{B.6})$$

Note that for both points, $(\boldsymbol{\omega}', \mathbf{0})$ and $(\boldsymbol{\omega}, \mathbf{K})$, the frequencies of the relative motion are the same:

$$\tilde{\omega}'^{(\alpha)} = \sqrt{(\omega'^{(\alpha)})^2 + \frac{NK'^{(\alpha)}}{m}} = \sqrt{(\omega^{(\alpha)})^2 + \frac{NK^{(\alpha)}}{m}} = \tilde{\omega}^{(\alpha)}, \quad \alpha = 1, \dots, n. \quad (\text{B.7})$$

Hence, the energies must be equal:

$$E_{(\vec{0}, \vec{\nu}_2, \dots, \vec{\nu}_N)}^{(\boldsymbol{\omega}, \mathbf{K})} = E_{(\vec{0}, \vec{\nu}_2, \dots, \vec{\nu}_N)}^{(\boldsymbol{\omega}', \mathbf{0})}, \quad \forall \vec{\nu}_2, \dots, \vec{\nu}_N. \quad (\text{B.8})$$

Furthermore, using Eqs. (B.7) and (B.1) one recognises that the eigenspaces of $(\boldsymbol{\omega}', \mathbf{0})$ and $(\boldsymbol{\omega}, \mathbf{K})$ are equivalent up to multiplication by a Gaussian factor $G^{(\boldsymbol{\omega}, \mathbf{K})} = \exp \left[-\frac{N}{2} \sum_{\alpha=1}^n \left(\frac{1}{l'^{(\alpha)2}} - \frac{1}{l^{(\alpha)2}} \right) (X^{(\alpha)})^2 \right]$ (see Ref. [83]):

$$\mathcal{H}_{[(\vec{0}, \vec{\nu}_2, \dots, \vec{\nu}_N)]}^{(\boldsymbol{\omega}, \mathbf{K})} = G^{(\boldsymbol{\omega}, \mathbf{K})} \mathcal{H}_{[(\vec{0}, \vec{\nu}_2, \dots, \vec{\nu}_N)]}^{(\boldsymbol{\omega}', \mathbf{0})}, \quad (\text{B.9})$$

with $X^{(\alpha)} \equiv y_1^{(\alpha)} \equiv \frac{1}{N} (x_1^{(\alpha)} + \dots + x_N^{(\alpha)})$ the center of mass coordinate in α -direction.

3. The ground state for the coupling parameters $(\boldsymbol{\omega}', \mathbf{K}') = (\tilde{\boldsymbol{\omega}}, \mathbf{0})$ of noninteracting fermions is simply given by the Slater determinant of N different single-particle states with lowest possible energy eigenvalues. These single-particle states are solutions of the Schrödinger equation for the single-harmonic oscillator in n -spatial dimensions, i.e. they are n -dimensional Hermite functions $\phi_{\boldsymbol{\mu}}^{(\vec{l})}(\vec{x}) \equiv \prod_{\alpha=1}^n \varphi_{\mu^{(\alpha)}}^{(\vec{l}^{(\alpha)})}(x^{(\alpha)})$ with energies $\varepsilon_{\boldsymbol{\mu}} = \sum_{\alpha=1}^n (\mu^{(\alpha)} + \frac{1}{2}) \hbar \tilde{\omega}^{(\alpha)}$. The quantum numbers $\boldsymbol{\mu}_1 = \mathbf{0}, \dots, \boldsymbol{\mu}_N$ of the N lowest energies $\varepsilon_{\boldsymbol{\mu}}$ are referred to as 'configuration' of the ground state

$$\Psi_{gs}^{(\tilde{\boldsymbol{\omega}}, \mathbf{0})} = \phi_{\boldsymbol{\mu}_1}^{(\vec{l})} \wedge \dots \wedge \phi_{\boldsymbol{\mu}_N}^{(\vec{l})}. \quad (\text{B.10})$$

Note that due to the structure of this ground state, the frequencies $\tilde{\omega}^{(\alpha)}$ must be pairwise distinct and therefore the ground state associated with $(\tilde{\boldsymbol{\omega}}, \mathbf{0})$ is unique for arbitrary points $(\boldsymbol{\omega}, \mathbf{K}) \in \Omega$.

4. Bringing together Eqs. (B.10), (B.8) and (B.9), we can determine the ground state for any point $(\boldsymbol{\omega}, \mathbf{K})$ of the coupling parameter space:

$$\Psi_{gs}^{(\tilde{\boldsymbol{\omega}}, \mathbf{0})} \in \mathcal{H}_{[(\vec{0}, \vec{\nu}_2, \dots, \vec{\nu}_N)]}^{(\tilde{\boldsymbol{\omega}}, \mathbf{0})} \Leftrightarrow \Psi_{gs}^{(\boldsymbol{\omega}, \mathbf{K})} \in \mathcal{H}_{[(\vec{0}, \vec{\nu}_2, \dots, \vec{\nu}_N)]}^{(\boldsymbol{\omega}, \mathbf{K})}. \quad (\text{B.11})$$

Therefore, we have

$$\mathcal{A}_N \mathcal{H}_{[(\vec{0}, \vec{\nu}_2, \dots, \vec{\nu}_N)]}^{(\boldsymbol{\omega}, \mathbf{K})} = \mathcal{A}_N G^{(\boldsymbol{\omega}, \mathbf{K})} \mathcal{H}_{[(\vec{0}, \vec{\nu}_2, \dots, \vec{\nu}_N)]}^{(\tilde{\boldsymbol{\omega}}, \mathbf{0})} = G^{(\boldsymbol{\omega}, \mathbf{K})} \mathcal{A}_N \mathcal{H}_{[(\vec{0}, \vec{\nu}_2, \dots, \vec{\nu}_N)]}^{(\tilde{\boldsymbol{\omega}}, \mathbf{0})}, \quad (\text{B.12})$$

which implies

$$\Psi_{gs}^{(\omega, \mathbf{K})} = G^{(\omega, \mathbf{K})} \Psi_{gs}^{(\tilde{\omega}, \mathbf{0})}. \quad (\text{B.13})$$

This finalises the proof of Thm. 3. We note that only the fermionic ground state can be derived in this manner. For excited states, this is not possible since the center-of-mass motion might carry excitations and so $\vec{\nu}_1 = 0$ cannot be assumed.

B.2 Derivation of the fermionic 1-RDO of N -Harmonium in n spatial dimensions

Starting with the general form of the ground state wave function of N -Harmonium in n spatial dimensions, Eq. (3.5), the partial trace over $(N - 1)$ fermions of the N -particle density operator $\rho_N = \Psi^* \Psi$ will be computed by integrating ρ_N over the particle positions $\vec{x}_i \in \mathbb{R}^n$ with labels $i = 2, \dots, N$. Using the Hubbard-Stratonovich relation for each spatial dimension $\gamma = 1, \dots, n$,

$$\begin{aligned} & \exp[a^{(\gamma)}(x_1^{(\gamma)} + \dots + x_N^{(\gamma)})^2] \\ &= \sqrt{\frac{a^{(\gamma)}}{\pi}} \int dy^{(\gamma)} \exp[-a^{(\gamma)}(y^{(\gamma)})^2 + 2a^{(\gamma)}y^{(\gamma)}(x_1^{(\gamma)} + \dots + x_N^{(\gamma)})], \end{aligned} \quad (\text{B.14})$$

one gets (see Ref. [83])

$$\begin{aligned} & \rho_1^{(f)}(\vec{x}; \vec{x}') \quad (\text{B.15}) \\ &= |\mathcal{N}|^2 \cdot \underbrace{\prod_{\gamma=1}^d \left(\exp \left[\left(\frac{1}{N^2} B^{(\gamma)} + C^{(\gamma)} - A^{(\gamma)} \right) ((x^{(\gamma)})^2 + (x'^{(\gamma)})^2) + 2C_N^{(\gamma)} x^{(\gamma)} x'^{(\gamma)} \right] \right)}_{\rho_1^{(b)}(\vec{x}; \vec{x}')} \\ & \times \underbrace{\sum_{i=1}^N \left(\prod_{\gamma=1}^d \int du_\gamma \left\{ \frac{e^{-u_\gamma^2} H_{\mu_i^{(\gamma)}}(p_\gamma u_\gamma + r_\gamma(x^{(\gamma)}, x'^{(\gamma)})) H_{\mu_i^{(\gamma)}}(p_\gamma u_\gamma + r_\gamma(x'^{(\gamma)}, x^{(\gamma)}))}{2\mu_i^{(\gamma)} (\mu_i^{(\gamma)})!} \right\} \right)}_{\equiv F(\vec{x}; \vec{x}')} \end{aligned}$$

In this expression, $H_{\mu_i^{(\gamma)}}$ denotes the Hermite polynomial of degree $\mu_i^{(\gamma)}$, where $\{\boldsymbol{\mu}_i\}_{i=1}^N$ is the set of quantum number vectors introduced in Section 3.1. The quantities

$A^{(\gamma)}, B^{(\gamma)}, C^{(\gamma)}, p$ and $r(\cdot, \cdot)$ are given by

$$A^{(\gamma)} = \frac{1}{2(\tilde{l}^{(\gamma)})^2}, \quad (\text{B.16})$$

$$B^{(\gamma)} = \frac{N}{2} \left(\frac{1}{(\tilde{l}^{(\gamma)})^2} - \frac{1}{(l^{(\gamma)})^2} \right), \quad (\text{B.17})$$

$$C^{(\gamma)} = \frac{(N-1)(B^{(\gamma)})^2}{2N^2(N^2A^{(\gamma)} - (N-1)B^{(\gamma)})}, \quad (\text{B.18})$$

$$p_\gamma = \sqrt{\frac{B^{(\gamma)}}{N^2A^{(\gamma)} - B^{(\gamma)}(N-1)}} \quad \text{and} \quad (\text{B.19})$$

$$r_\gamma(v, w) = \sqrt{2A^{(\gamma)}} \left(v - \frac{B^{(\gamma)}}{2(N^2A^{(\gamma)} - (N-1)B^{(\gamma)})}(v+w) \right), \quad (\text{B.20})$$

where we suppressed the index N of $A^{(\gamma)}, B^{(\gamma)}$ and $C^{(\gamma)}$. Again, $l^{(\gamma)}$ and $\tilde{l}^{(\gamma)}$ denote the length scales in γ -direction for the center-of-mass and the relative motion, respectively.

The 1-RDO associated with the ground state of Harmonium for spinful fermions can be derived by tracing out spin and spatial degrees of freedom by applying the same ideas to the spatial part as in the case of fully spin-polarised Harmonium Eq. (B.15):

$$\begin{aligned} & \rho_1^{(f)}(\vec{x}, \sigma; \vec{x}', \sigma') \\ &= |\mathcal{N}|^2 \cdot \underbrace{\prod_{\gamma=1}^d \left(\exp \left[\left(\frac{1}{N^2} B^{(\gamma)} + C^{(\gamma)} - A^{(\gamma)} \right) \left((x^{(\gamma)})^2 + (x'^{(\gamma)})^2 \right) + 2C^{(\gamma)} x^{(\gamma)} x'^{(\gamma)} \right] \right)}_{\rho_1^{(b)}(\vec{x}; \vec{x}')} \\ & \left[\underbrace{\sum_{i=1}^{N^\uparrow} \left(\prod_{\gamma=1}^d \int du_\gamma \left\{ \frac{e^{-u_\gamma^2} H_{\mu_i^\uparrow(\gamma)}(p_\gamma u_\gamma + r_\gamma(x^{(\gamma)}, x'^{(\gamma)})) H_{\mu_i^\uparrow(\gamma)}(p_\gamma u_\gamma + r_\gamma(x'^{(\gamma)}, x^{(\gamma)}))}{2^{\mu_i^\uparrow(\gamma)} (\mu_i^\uparrow(\gamma))!} \right\} \right)}_{\equiv F^\uparrow(\vec{x}; \vec{x}')} |\uparrow\rangle \langle \uparrow| \right. \\ & \left. + \sum_{i=1}^{N^\downarrow} \left(\prod_{\gamma=1}^d \int du_\gamma \left\{ \frac{e^{-u_\gamma^2} H_{\mu_i^\downarrow(\gamma)}(p_\gamma u_\gamma + r_\gamma(x^{(\gamma)}, x^{(\gamma)})) H_{\mu_i^\downarrow(\gamma)}(p_\gamma u_\gamma + r_\gamma(x'^{(\gamma)}, x^{(\gamma)}))}{2^{\mu_i^\downarrow(\gamma)} (\mu_i^\downarrow(\gamma))!} \right\} \right) |\downarrow\rangle \langle \downarrow| \right]. \end{aligned} \quad (\text{B.21})$$

In this expression, the $\mu_i^\uparrow$ and $\mu_j^\downarrow$ quantum number vectors represent the set of particles with spins parallel and antiparallel to the external magnetic field.

B.3 Natural occupation numbers of the 3-Harmonium ground state in one dimension

For completeness, we include the natural occupation numbers of the fermionic one-dimensional 3-Harmonium ground state presented in Ref. [87]. Up to corrections of the order $\mathcal{O}(\delta^{10})$, these NONs are given by:

$$\begin{aligned}
1 - \lambda_1 &= \frac{40}{729}\delta^6 - \frac{1390}{59049}\delta^8 + \mathcal{O}(\delta^{10}), \\
1 - \lambda_2 &= \frac{2}{9}\delta^4 - \frac{232}{729}\delta^6 + \frac{3926}{10935}\delta^8 + \mathcal{O}(\delta^{10}), \\
1 - \lambda_3 &= \frac{2}{9}\delta^4 - \frac{64}{243}\delta^6 + \frac{81902}{295245}\delta^8 + \mathcal{O}(\delta^{10}), \\
\lambda_4 &= \frac{2}{9}\delta^4 - \frac{64}{243}\delta^6 + \frac{73802}{295245}\delta^8 + \mathcal{O}(\delta^{10}), \\
\lambda_5 &= \frac{2}{9}\delta^4 - \frac{232}{729}\delta^6 + \frac{3976}{10935}\delta^8 + \mathcal{O}(\delta^{10}), \\
\lambda_6 &= \frac{40}{729}\delta^6 - \frac{2200}{59049}\delta^8 + \mathcal{O}(\delta^{10}), \\
\lambda_7 &= \frac{80}{2187}\delta^8 + \mathcal{O}(\delta^{10}), \\
\lambda_k &= \mathcal{O}(\delta^{2k-6}), \quad \text{for } k \geq 8,
\end{aligned} \tag{B.22}$$

where the coupling parameter δ is defined as in Eq. (3.26).

Appendix C

Transformation of N -particle states between Momentum- and Position-space

In this appendix, we derive the explicit form of the transformation of N -particle states from momentum to position-space and vice versa. Let $\{|j\rangle_x\}_{j=0}^{d-1}$ denote an orthonormalised one-particle position-space basis, where d represents the dimension of the one-particle Hilbert space $\mathcal{H}_1^{(d)}$. The related 1-particle momentum-space basis is derived by a discrete Fourier transformation:

$$|k\rangle_p = \frac{1}{\sqrt{d}} \sum_{j=0}^{d-1} e^{+2\pi i j k / d} |j\rangle_x. \quad (\text{C.1})$$

Under this convention, the corresponding back transformation becomes:

$$|j\rangle_x = \frac{1}{\sqrt{d}} \sum_{k=0}^{d-1} e^{-2\pi i j k / d} |k\rangle_p. \quad (\text{C.2})$$

An orthonormalised basis of the Hilbert space of N indistinguishable particles is given by Slater determinants or permanents of orthonormal single-particle states:

$$|k_1, k_2, \dots, k_N\rangle = A \sum_{\sigma \in S_N} (\pm 1)^{\text{sign}[\sigma]} |k_{\sigma(1)}\rangle \otimes |k_{\sigma(2)}\rangle \otimes \dots \otimes |k_{\sigma(N)}\rangle, \quad (\text{C.3})$$

where the plus sign refers to bosonic permanents, the minus sign to fermionic determinants and S_N represents the group of all permutations of N elements. The normalisation constant A depends on the multiplicities of the levels k_i in $|k_1, k_2, \dots, k_N\rangle$. Using Eq. (C.1), we can now decompose a momentum-space Slater permanent (de-

terminant) into a linear superposition of position-space states:

$$\begin{aligned}
|k_1, k_2, \dots, k_N\rangle_p &= A \sum_{\sigma \in S_N} (\pm 1)^{\text{sign}[\sigma]} |k_{\sigma(1)}\rangle_p \otimes |k_{\sigma(2)}\rangle_p \otimes \dots \otimes |k_{\sigma(N)}\rangle_p \\
&= A \sum_{\sigma \in S_N} (\pm 1)^{\text{sign}[\sigma]} \left[\left(\frac{1}{\sqrt{d}} \sum_{n_1=0}^{d-1} e^{+2\pi i n_1 k_{\sigma(1)}/d} |n_1\rangle_x \right) \otimes \right. \\
&\quad \otimes \left(\frac{1}{\sqrt{d}} \sum_{n_2=0}^{d-1} e^{+2\pi i n_2 k_{\sigma(2)}/d} |n_2\rangle_x \right) \otimes \dots \\
&\quad \left. \dots \otimes \left(\frac{1}{\sqrt{d}} \sum_{n_N=0}^{d-1} e^{+2\pi i n_N k_{\sigma(N)}/d} |n_N\rangle_x \right) \right]. \tag{C.4}
\end{aligned}$$

For some arbitrary but fixed permutation $\tau \in S_N$, each sum over n_i will be equal to a sum over $n_{\tau(i)}$:

$$\begin{aligned}
|k_1, k_2, \dots, k_N\rangle_p &= A \sum_{\sigma \in S_N} (\pm 1)^{\text{sign}[\sigma]} \left[\left(\frac{1}{\sqrt{d}} \sum_{n_{\tau(1)}=0}^{d-1} e^{+2\pi i n_{\tau(1)} k_{\sigma(1)}/d} |n_{\tau(1)}\rangle_x \right) \otimes \right. \\
&\quad \otimes \left(\frac{1}{\sqrt{d}} \sum_{n_{\tau(2)}=0}^{d-1} e^{+2\pi i n_{\tau(2)} k_{\sigma(2)}/d} |n_{\tau(2)}\rangle_x \right) \otimes \dots \\
&\quad \left. \dots \otimes \left(\frac{1}{\sqrt{d}} \sum_{n_{\tau(N)}=0}^{d-1} e^{+2\pi i n_{\tau(N)} k_{\sigma(N)}/d} |n_{\tau(N)}\rangle_x \right) \right]. \tag{C.5}
\end{aligned}$$

For each summand in the squared brackets we can therefore choose $\tau = \sigma$ yielding:

$$\begin{aligned}
|k_1, k_2, \dots, k_N\rangle_p &= \frac{A}{\sqrt{d^N}} \\
&\times \sum_{\sigma \in S_N} (\pm 1)^{\text{sign}[\sigma]} \left[\sum_{n_{\sigma(1)}=0}^{d-1} \dots \sum_{n_{\sigma(N)}=0}^{d-1} e^{\frac{2\pi i}{d}(n_{\sigma(1)} k_{\sigma(1)} + \dots + n_{\sigma(N)} k_{\sigma(N)})} |n_{\sigma(1)}\rangle_x \otimes \dots \otimes |n_{\sigma(N)}\rangle_x \right]. \tag{C.6}
\end{aligned}$$

It is now crucial to note that all N sums over $n_{\sigma(i)}$, $i = 1 \dots N$ commute for some arbitrary but fixed σ . Therefore, it is possible to re-order and write them as a series of sums over n_i , $i = 1 \dots N$ for each fixed σ independently:

$$\begin{aligned}
|k_1, k_2, \dots, k_N\rangle_p &= \frac{A}{\sqrt{d^N}} \\
&\times \sum_{\sigma \in S_N} (\pm 1)^{\text{sign}[\sigma]} \left[\sum_{n_1=0}^{d-1} \dots \sum_{n_N=0}^{d-1} e^{+\frac{2\pi i}{d}(n_{\sigma(1)} k_{\sigma(1)} + \dots + n_{\sigma(N)} k_{\sigma(N)})} |n_{\sigma(1)}\rangle_x \otimes \dots \otimes |n_{\sigma(N)}\rangle_x \right]. \tag{C.7}
\end{aligned}$$

Further, the outer sum over all permutations $\sigma \in S_N$ commutes with each single sum over n_i :

$$\begin{aligned} |k_1, k_2, \dots, k_N\rangle_p &= \frac{A}{\sqrt{d^N}} \\ &\times \sum_{n_1=0}^{d-1} \dots \sum_{n_N=0}^{d-1} \left[\sum_{\sigma \in S_N} (\pm 1)^{\text{sign}[\sigma]} e^{+\frac{2\pi i}{d}(n_{\sigma(1)}k_{\sigma(1)} + \dots + n_{\sigma(N)}k_{\sigma(N)})} |n_{\sigma(1)}\rangle_x \otimes \dots \otimes |n_{\sigma(N)}\rangle_x \right]. \end{aligned} \quad (\text{C.8})$$

Since the exponential function remains invariant under simultaneous permutation of the k_i and n_i , we can carry out the sum over σ :

$$|k_1, k_2, \dots, k_N\rangle_p = \sum_{n_1=0}^{d-1} \dots \sum_{n_N=0}^{d-1} \left[\frac{1}{A\sqrt{d^N}} e^{+\frac{2\pi i}{d}(n_1k_1 + \dots + n_Nk_N)} |n_1, n_2, \dots, n_N\rangle_x \right], \quad (\text{C.9})$$

where $|n_1, n_2, \dots, n_N\rangle_x$ represents the normalised Slater determinant or permanent of single-particle position-space states.

Note that the general back transformation from momentum to position space is mediated via:

$$|j_1, j_2, \dots, j_N\rangle_x = A' \sum_{k_1=0}^{d-1} \dots \sum_{k_N=0}^{d-1} \left[\frac{1}{\sqrt{d^N}} e^{-\frac{2\pi i}{d}(k_1j_1 + \dots + k_Nj_N)} |k_1, k_2, \dots, k_N\rangle_p \right], \quad (\text{C.10})$$

which only differs from the transformation (C.9) by the negative sign in the exponential function.

In the case of N fermions only Slater determinants with $n_i \neq n_j$ for $i \neq j$ will not vanish in Eq. (C.9). Let $\mathbb{P}_d^N$ again denote the set of all N -subsets of $\{1, 2, \dots, d\}$. The fourier transformed state can then be written as:

$$|k_1, k_2, \dots, k_N\rangle_p = \sum_{\mathbf{n} \in \mathbb{P}_d^N} \sum_{\sigma(\mathbf{n}) \in S_N} \left[\frac{1}{\sqrt{d^N}} e^{+\frac{2\pi i}{d} \mathbf{k} \cdot \sigma(\mathbf{n})} (-1)^{\text{sign}[\sigma]} |n_1, n_2, \dots, n_N\rangle_x \right]; \quad (\text{C.11})$$

the sum over $\sigma(\mathbf{n}) \in S_N$ represents the sum over all permutations of elements of some fixed N -subset $\mathbf{n} \in \mathbb{P}_d^N$. A list of examples can be found in Tables C.1 and C.2.

In the case of hardcore bosons, N -particle momentum-space permanents of the form $|k_1, k_2, \dots, k_N\rangle_p$ generally violate the hardcore boson constraint since the sum in Eq. (C.9) also comprises of position-space N -particle states with some occupancies larger than one, e.g. $|0, 0, \dots\rangle_x$. We are therefore more interested in the expansion of $\hat{K} |k_1, \dots, k_N\rangle_p$, where $\hat{K}$ represents the projection operator onto the hardcore boson subspace (see Section 4.1). The projector clearly annihilates all terms but those with

all n_i distinct. This almost resembles the case of fermions up to the signature of permutations and therefore allows us to conclude that:

$$\hat{K} |k_1, k_2, \dots, k_N\rangle_p = A\sqrt{N!} \sum_{\mathbf{n} \in \mathbb{P}_d^N} \sum_{\sigma(\mathbf{n}) \in S_N} \left[\frac{1}{\sqrt{d^N}} e^{+\frac{2\pi i}{d} \mathbf{k} \cdot \sigma(\mathbf{n})} |n_1, n_2, \dots, n_N\rangle_x \right]. \quad (\text{C.12})$$

Examples of projected momentum-space hardcore boson states may be found in the Tables C.3-C.6.

$\hat{K} 0, 1\rangle_p$	$\frac{1}{\sqrt{3}}e^{-\frac{5i\pi}{6}} 0, 1\rangle_x + \frac{1}{\sqrt{3}}e^{\frac{5i\pi}{6}} 0, 2\rangle_x + \frac{1}{\sqrt{3}}i 1, 2\rangle_x$
$\hat{K} 0, 2\rangle_p$	$\frac{1}{\sqrt{3}}e^{\frac{5i\pi}{6}} 0, 1\rangle_x + \frac{1}{\sqrt{3}}e^{-\frac{5i\pi}{6}} 0, 2\rangle_x - \frac{1}{\sqrt{3}}i 1, 2\rangle_x$
$\hat{K} 1, 2\rangle_p$	$\frac{1}{\sqrt{3}}i 0, 1\rangle_x - \frac{1}{\sqrt{3}}i 0, 2\rangle_x + \frac{1}{\sqrt{3}}i 1, 2\rangle_x$

Table C.1: Expansion of momentum-space states in terms of position-space states of $N = 2$ fermions on $d = 3$ sites.

$\hat{K} 0, 1\rangle_p$	$\frac{e^{-\frac{3i\pi}{4}}}{2\sqrt{2}} 0, 1\rangle_x - \frac{1}{2} 0, 2\rangle_x + \frac{e^{\frac{3i\pi}{4}}}{2\sqrt{2}} 0, 3\rangle_x + \frac{e^{\frac{3i\pi}{4}}}{2\sqrt{2}} 1, 2\rangle_x + \frac{1}{2}i 1, 3\rangle_x + \frac{e^{\frac{i\pi}{4}}}{2\sqrt{2}} 2, 3\rangle_x$
$\hat{K} 0, 2\rangle_p$	$-\frac{1}{2} 0, 1\rangle_x - \frac{1}{2} 0, 3\rangle_x + \frac{1}{2} 1, 2\rangle_x - \frac{1}{2} 2, 3\rangle_x$
$\hat{K} 0, 3\rangle_p$	$\frac{e^{\frac{3i\pi}{4}}}{2\sqrt{2}} 0, 1\rangle_x - \frac{1}{2} 0, 2\rangle_x + \frac{e^{-\frac{3i\pi}{4}}}{2\sqrt{2}} 0, 3\rangle_x + \frac{e^{-\frac{3i\pi}{4}}}{2\sqrt{2}} 1, 2\rangle_x - \frac{1}{2}i 1, 3\rangle_x + \frac{e^{-\frac{i\pi}{4}}}{2\sqrt{2}} 2, 3\rangle_x$
$\hat{K} 1, 2\rangle_p$	$\frac{e^{\frac{3i\pi}{4}}}{2\sqrt{2}} 0, 1\rangle_x + \frac{1}{2} 0, 2\rangle_x + \frac{e^{-\frac{3i\pi}{4}}}{2\sqrt{2}} 0, 3\rangle_x + \frac{e^{-\frac{3i\pi}{4}}}{2\sqrt{2}} 1, 2\rangle_x + \frac{1}{2}i 1, 3\rangle_x + \frac{e^{-\frac{i\pi}{4}}}{2\sqrt{2}} 2, 3\rangle_x$
$\hat{K} 1, 3\rangle_p$	$\frac{1}{2}i 0, 1\rangle_x - \frac{1}{2}i 0, 3\rangle_x + \frac{1}{2}i 1, 2\rangle_x + \frac{1}{2}i 2, 3\rangle_x$
$\hat{K} 2, 3\rangle_p$	$\frac{e^{\frac{i\pi}{4}}}{2\sqrt{2}} 0, 1\rangle_x - \frac{1}{2} 0, 2\rangle_x + \frac{e^{-\frac{i\pi}{4}}}{2\sqrt{2}} 0, 3\rangle_x + \frac{e^{-\frac{i\pi}{4}}}{2\sqrt{2}} 1, 2\rangle_x + \frac{1}{2}i 1, 3\rangle_x + \frac{e^{-\frac{3i\pi}{4}}}{2\sqrt{2}} 2, 3\rangle_x$

Table C.2: Expansion of momentum-space states in terms of position-space states of $N = 2$ fermions on $d = 4$ sites.

$\hat{K} 0,0\rangle_p$	$\frac{1}{3}\sqrt{2} 0,1\rangle_x + \frac{1}{3}\sqrt{2} 0,2\rangle_x + \frac{1}{3}\sqrt{2} 1,2\rangle_x$
$\hat{K} 1,1\rangle_p$	$\frac{1}{3}\sqrt{2}e^{-\frac{2i\pi}{3}} 0,1\rangle_x + \frac{1}{3}\sqrt{2}e^{\frac{2i\pi}{3}} 0,2\rangle_x + \frac{1}{3}\sqrt{2} 1,2\rangle_x$
$\hat{K} 2,2\rangle_p$	$\frac{1}{3}\sqrt{2}e^{\frac{2i\pi}{3}} 0,1\rangle_x + \frac{1}{3}\sqrt{2}e^{-\frac{2i\pi}{3}} 0,2\rangle_x + \frac{1}{3}\sqrt{2} 1,2\rangle_x$
$\hat{K} 0,1\rangle_p$	$\frac{1}{3}e^{-\frac{i\pi}{3}} 0,1\rangle_x + \frac{1}{3}e^{\frac{i\pi}{3}} 0,2\rangle_x - \frac{1}{3} 1,2\rangle_x$
$\hat{K} 0,2\rangle_p$	$\frac{1}{3}e^{\frac{i\pi}{3}} 0,1\rangle_x + \frac{1}{3}e^{-\frac{i\pi}{3}} 0,2\rangle_x - \frac{1}{3} 1,2\rangle_x$
$\hat{K} 1,2\rangle_p$	$-\frac{1}{3} 0,1\rangle_x - \frac{1}{3} 0,2\rangle_x - \frac{1}{3} 1,2\rangle_x$

Table C.3: Expansion of $\hat{K}$ -projected momentum-space states in terms of position-space states of $N = 2$ hardcore bosons on $d = 3$ sites.

$\hat{K} 0,0\rangle_p$	$\frac{1}{2\sqrt{2}} 0,1\rangle_x + \frac{1}{2\sqrt{2}} 0,2\rangle_x + \frac{1}{2\sqrt{2}} 0,3\rangle_x + \frac{1}{2\sqrt{2}} 1,2\rangle_x + \frac{1}{2\sqrt{2}} 1,3\rangle_x + \frac{1}{2\sqrt{2}} 2,3\rangle_x$
$\hat{K} 1,1\rangle_p$	$-\frac{i}{2\sqrt{2}} 0,1\rangle_x - \frac{1}{2\sqrt{2}} 0,2\rangle_x + \frac{i}{2\sqrt{2}} 0,3\rangle_x + \frac{i}{2\sqrt{2}} 1,2\rangle_x + \frac{1}{2\sqrt{2}} 1,3\rangle_x - \frac{i}{2\sqrt{2}} 2,3\rangle_x$
$\hat{K} 2,2\rangle_p$	$-\frac{1}{2\sqrt{2}} 0,1\rangle_x + \frac{1}{2\sqrt{2}} 0,2\rangle_x - \frac{1}{2\sqrt{2}} 0,3\rangle_x - \frac{1}{2\sqrt{2}} 1,2\rangle_x + \frac{1}{2\sqrt{2}} 1,3\rangle_x - \frac{1}{2\sqrt{2}} 2,3\rangle_x$
$\hat{K} 3,3\rangle_p$	$\frac{i}{2\sqrt{2}} 0,1\rangle_x - \frac{1}{2\sqrt{2}} 0,2\rangle_x - \frac{i}{2\sqrt{2}} 0,3\rangle_x - \frac{i}{2\sqrt{2}} 1,2\rangle_x + \frac{1}{2\sqrt{2}} 1,3\rangle_x + \frac{i}{2\sqrt{2}} 2,3\rangle_x$
$\hat{K} 0,1\rangle_p$	$\frac{1}{2\sqrt{2}}e^{-\frac{i\pi}{4}} 0,1\rangle_x + \frac{1}{2\sqrt{2}}e^{\frac{i\pi}{4}} 0,3\rangle_x + \frac{1}{2\sqrt{2}}e^{-\frac{3i\pi}{4}} 1,2\rangle_x + \frac{1}{2\sqrt{2}}e^{\frac{3i\pi}{4}} 2,3\rangle_x$
$\hat{K} 0,2\rangle_p$	$\frac{1}{2} 0,2\rangle_x - \frac{1}{2} 1,3\rangle_x$
$\hat{K} 0,3\rangle_p$	$\frac{1}{2\sqrt{2}}e^{\frac{i\pi}{4}} 0,1\rangle_x + \frac{1}{2\sqrt{2}}e^{-\frac{i\pi}{4}} 0,3\rangle_x + \frac{1}{2\sqrt{2}}e^{\frac{3i\pi}{4}} 1,2\rangle_x + \frac{1}{2\sqrt{2}}e^{-\frac{3i\pi}{4}} 2,3\rangle_x$
$\hat{K} 1,2\rangle_p$	$\frac{1}{2\sqrt{2}}e^{-\frac{3i\pi}{4}} 0,1\rangle_x + \frac{1}{2\sqrt{2}}e^{\frac{3i\pi}{4}} 0,3\rangle_x + \frac{1}{2\sqrt{2}}e^{-\frac{i\pi}{4}} 1,2\rangle_x + \frac{1}{2\sqrt{2}}e^{\frac{i\pi}{4}} 2,3\rangle_x$
$\hat{K} 1,3\rangle_p$	$-\frac{1}{2} 0,2\rangle_x - \frac{1}{2} 1,3\rangle_x$
$\hat{K} 2,3\rangle_p$	$\frac{1}{2\sqrt{2}}e^{\frac{3i\pi}{4}} 0,1\rangle_x + \frac{1}{2\sqrt{2}}e^{-\frac{3i\pi}{4}} 0,3\rangle_x + \frac{1}{2\sqrt{2}}e^{\frac{i\pi}{4}} 1,2\rangle_x + \frac{1}{2\sqrt{2}}e^{-\frac{i\pi}{4}} 2,3\rangle_x$

Table C.4: Expansion of $\hat{K}$ -projected momentum-space states in terms of position-space states of $N = 2$ hardcore bosons on $d = 4$ sites.

$\hat{K} 0,0,0\rangle_p$	$+\frac{1}{6} 0,1,2\rangle_x + \frac{1}{6} 0,1,3\rangle_x + \frac{1}{6} 0,1,4\rangle_x + \frac{1}{6} 0,1,5\rangle_x + \frac{1}{6} 0,2,3\rangle_x$ $+\frac{1}{6} 0,2,4\rangle_x + \frac{1}{6} 0,2,5\rangle_x + \frac{1}{6} 0,3,4\rangle_x + \frac{1}{6} 0,3,5\rangle_x + \frac{1}{6} 0,4,5\rangle_x$ $+\frac{1}{6} 1,2,3\rangle_x + \frac{1}{6} 1,2,4\rangle_x + \frac{1}{6} 1,2,5\rangle_x + \frac{1}{6} 1,3,4\rangle_x + \frac{1}{6} 1,3,5\rangle_x$ $+\frac{1}{6} 1,4,5\rangle_x + \frac{1}{6} 2,3,4\rangle_x + \frac{1}{6} 2,3,5\rangle_x + \frac{1}{6} 2,4,5\rangle_x + \frac{1}{6} 3,4,5\rangle_x$
$\hat{K} 1,1,1\rangle_p$	$-\frac{1}{6} 0,1,2\rangle_x + \frac{1}{6}e^{\frac{2i\pi}{3}} 0,1,3\rangle_x + \frac{1}{6}e^{\frac{i\pi}{3}} 0,1,4\rangle_x + \frac{1}{6} 0,1,5\rangle_x + \frac{1}{6}e^{\frac{i\pi}{3}} 0,2,3\rangle_x$ $+\frac{1}{6} 0,2,4\rangle_x + \frac{1}{6}e^{-\frac{i\pi}{3}} 0,2,5\rangle_x + \frac{1}{6}e^{-\frac{i\pi}{3}} 0,3,4\rangle_x + \frac{1}{6}e^{-\frac{2i\pi}{3}} 0,3,5\rangle_x - \frac{1}{6} 0,4,5\rangle_x$ $+\frac{1}{6} 1,2,3\rangle_x + \frac{1}{6}e^{-\frac{i\pi}{3}} 1,2,4\rangle_x + \frac{1}{6}e^{-\frac{2i\pi}{3}} 1,2,5\rangle_x + \frac{1}{6}e^{-\frac{2i\pi}{3}} 1,3,4\rangle_x - \frac{1}{6} 1,3,5\rangle_x$ $+\frac{1}{6}e^{\frac{2i\pi}{3}} 1,4,5\rangle_x - \frac{1}{6} 2,3,4\rangle_x + \frac{1}{6}e^{\frac{2i\pi}{3}} 2,3,5\rangle_x + \frac{1}{6}e^{\frac{i\pi}{3}} 2,4,5\rangle_x + \frac{1}{6} 3,4,5\rangle_x$
$\hat{K} 2,2,2\rangle_p$	$+\frac{1}{6} 0,1,2\rangle_x + \frac{1}{6}e^{-\frac{2i\pi}{3}} 0,1,3\rangle_x + \frac{1}{6}e^{\frac{2i\pi}{3}} 0,1,4\rangle_x + \frac{1}{6} 0,1,5\rangle_x + \frac{1}{6}e^{\frac{2i\pi}{3}} 0,2,3\rangle_x$ $+\frac{1}{6} 0,2,4\rangle_x + \frac{1}{6}e^{-\frac{2i\pi}{3}} 0,2,5\rangle_x + \frac{1}{6}e^{-\frac{2i\pi}{3}} 0,3,4\rangle_x + \frac{1}{6}e^{\frac{2i\pi}{3}} 0,3,5\rangle_x + \frac{1}{6} 0,4,5\rangle_x$ $+\frac{1}{6} 1,2,3\rangle_x + \frac{1}{6}e^{-\frac{2i\pi}{3}} 1,2,4\rangle_x + \frac{1}{6}e^{\frac{2i\pi}{3}} 1,2,5\rangle_x + \frac{1}{6}e^{\frac{2i\pi}{3}} 1,3,4\rangle_x + \frac{1}{6} 1,3,5\rangle_x$ $+\frac{1}{6}e^{-\frac{2i\pi}{3}} 1,4,5\rangle_x + \frac{1}{6} 2,3,4\rangle_x + \frac{1}{6}e^{-\frac{2i\pi}{3}} 2,3,5\rangle_x + \frac{1}{6}e^{\frac{2i\pi}{3}} 2,4,5\rangle_x + \frac{1}{6} 3,4,5\rangle_x$
$\hat{K} 3,3,3\rangle_p$	$-\frac{1}{6} 0,1,2\rangle_x + \frac{1}{6} 0,1,3\rangle_x - \frac{1}{6} 0,1,4\rangle_x + \frac{1}{6} 0,1,5\rangle_x - \frac{1}{6} 0,2,3\rangle_x$ $+\frac{1}{6} 0,2,4\rangle_x - \frac{1}{6} 0,2,5\rangle_x - \frac{1}{6} 0,3,4\rangle_x + \frac{1}{6} 0,3,5\rangle_x - \frac{1}{6} 0,4,5\rangle_x$ $+\frac{1}{6} 1,2,3\rangle_x - \frac{1}{6} 1,2,4\rangle_x + \frac{1}{6} 1,2,5\rangle_x + \frac{1}{6} 1,3,4\rangle_x - \frac{1}{6} 1,3,5\rangle_x$ $+\frac{1}{6} 1,4,5\rangle_x - \frac{1}{6} 2,3,4\rangle_x + \frac{1}{6} 2,3,5\rangle_x - \frac{1}{6} 2,4,5\rangle_x + \frac{1}{6} 3,4,5\rangle_x$
$\hat{K} 4,4,4\rangle_p$	$\frac{1}{6} 0,1,2\rangle_x + \frac{1}{6}e^{\frac{2i\pi}{3}} 0,1,3\rangle_x + \frac{1}{6}e^{-\frac{2i\pi}{3}} 0,1,4\rangle_x + \frac{1}{6} 0,1,5\rangle_x + \frac{1}{6}e^{-\frac{2i\pi}{3}} 0,2,3\rangle_x$ $+\frac{1}{6} 0,2,4\rangle_x + \frac{1}{6}e^{\frac{2i\pi}{3}} 0,2,5\rangle_x + \frac{1}{6}e^{\frac{2i\pi}{3}} 0,3,4\rangle_x + \frac{1}{6}e^{-\frac{2i\pi}{3}} 0,3,5\rangle_x + \frac{1}{6} 0,4,5\rangle_x$ $+\frac{1}{6} 1,2,3\rangle_x + \frac{1}{6}e^{\frac{2i\pi}{3}} 1,2,4\rangle_x + \frac{1}{6}e^{-\frac{2i\pi}{3}} 1,2,5\rangle_x + \frac{1}{6}e^{-\frac{2i\pi}{3}} 1,3,4\rangle_x + \frac{1}{6} 1,3,5\rangle_x$ $+\frac{1}{6}e^{\frac{2i\pi}{3}} 1,4,5\rangle_x + \frac{1}{6} 2,3,4\rangle_x + \frac{1}{6}e^{\frac{2i\pi}{3}} 2,3,5\rangle_x + \frac{1}{6}e^{-\frac{2i\pi}{3}} 2,4,5\rangle_x + \frac{1}{6} 3,4,5\rangle_x$
$\hat{K} 5,5,5\rangle_p$	$-\frac{1}{6} 0,1,2\rangle_x + \frac{1}{6}e^{-\frac{2i\pi}{3}} 0,1,3\rangle_x + \frac{1}{6}e^{-\frac{i\pi}{3}} 0,1,4\rangle_x + \frac{1}{6} 0,1,5\rangle_x + \frac{1}{6}e^{-\frac{i\pi}{3}} 0,2,3\rangle_x$ $+\frac{1}{6} 0,2,4\rangle_x + \frac{1}{6}e^{\frac{i\pi}{3}} 0,2,5\rangle_x + \frac{1}{6}e^{\frac{i\pi}{3}} 0,3,4\rangle_x + \frac{1}{6}e^{\frac{2i\pi}{3}} 0,3,5\rangle_x - \frac{1}{6} 0,4,5\rangle_x$ $+\frac{1}{6} 1,2,3\rangle_x + \frac{1}{6}e^{\frac{i\pi}{3}} 1,2,4\rangle_x + \frac{1}{6}e^{\frac{2i\pi}{3}} 1,2,5\rangle_x + \frac{1}{6}e^{\frac{2i\pi}{3}} 1,3,4\rangle_x - \frac{1}{6} 1,3,5\rangle_x$ $+\frac{1}{6}e^{-\frac{2i\pi}{3}} 1,4,5\rangle_x - \frac{1}{6} 2,3,4\rangle_x + \frac{1}{6}e^{-\frac{2i\pi}{3}} 2,3,5\rangle_x + \frac{1}{6}e^{-\frac{i\pi}{3}} 2,4,5\rangle_x + \frac{1}{6} 3,4,5\rangle_x$

Table C.5: Expansion of $\hat{K}$ -projected momentum-space states in terms of position-space states of $N = 3$ hardcore bosons on $d = 6$ sites.

$\hat{K} 0,0,1\rangle_p$	$ \begin{aligned} & + \frac{1}{3\sqrt{3}}e^{-\frac{i\pi}{3}} 0,1,2\rangle_x + \frac{1}{6\sqrt{3}}e^{-\frac{i\pi}{3}} 0,1,3\rangle_x + \frac{1}{6\sqrt{3}} 0,1,4\rangle_x + \frac{1}{3\sqrt{3}} 0,1,5\rangle_x \\ & + \frac{1}{6\sqrt{3}}e^{-\frac{2i\pi}{3}} 0,2,3\rangle_x + \frac{1}{6\sqrt{3}} 0,2,5\rangle_x + \frac{1}{6\sqrt{3}}e^{\frac{2i\pi}{3}} 0,3,4\rangle_x + \frac{1}{6\sqrt{3}}e^{\frac{i\pi}{3}} 0,3,5\rangle_x \\ & + \frac{1}{3\sqrt{3}}e^{\frac{i\pi}{3}} 0,4,5\rangle_x + \frac{1}{3\sqrt{3}}e^{-\frac{2i\pi}{3}} 1,2,3\rangle_x + \frac{1}{6\sqrt{3}}e^{-\frac{2i\pi}{3}} 1,2,4\rangle_x \\ & + \frac{1}{6\sqrt{3}}e^{-\frac{i\pi}{3}} 1,2,5\rangle_x - \frac{1}{6\sqrt{3}} 1,3,4\rangle_x + \frac{1}{6\sqrt{3}}e^{\frac{i\pi}{3}} 1,4,5\rangle_x - \frac{1}{3\sqrt{3}} 2,3,4\rangle_x \\ & - \frac{1}{6\sqrt{3}} 2,3,5\rangle_x + \frac{1}{6\sqrt{3}}e^{\frac{2i\pi}{3}} 2,4,5\rangle_x + \frac{1}{3\sqrt{3}}e^{\frac{2i\pi}{3}} 3,4,5\rangle_x \end{aligned} $
$\hat{K} 0,0,2\rangle_p$	$ \begin{aligned} & \frac{1}{6}e^{-\frac{i\pi}{6}} 0,1,3\rangle_x - \frac{1}{6}i 0,1,4\rangle_x + \frac{1}{6}e^{\frac{i\pi}{6}} 0,2,3\rangle_x + \frac{1}{6}i 0,2,5\rangle_x + \frac{1}{6}e^{-\frac{i\pi}{6}} 0,3,4\rangle_x \\ & + \frac{1}{6}e^{\frac{i\pi}{6}} 0,3,5\rangle_x + \frac{1}{6}e^{-\frac{5i\pi}{6}} 1,2,4\rangle_x + \frac{1}{6}e^{\frac{5i\pi}{6}} 1,2,5\rangle_x - \frac{1}{6}i 1,3,4\rangle_x \\ & + \frac{1}{6}e^{-\frac{5i\pi}{6}} 1,4,5\rangle_x + \frac{1}{6}i 2,3,5\rangle_x + \frac{1}{6}e^{\frac{5i\pi}{6}} 2,4,5\rangle_x \end{aligned} $
$\hat{K} 0,1,3\rangle_p$	$ \begin{aligned} & \frac{1}{3\sqrt{6}}e^{-\frac{i\pi}{3}} 0,1,2\rangle_x - \frac{1}{3\sqrt{6}} 0,1,3\rangle_x + \frac{1}{3\sqrt{6}}e^{-\frac{i\pi}{3}} 0,1,4\rangle_x - \frac{1}{3\sqrt{6}} 0,1,5\rangle_x \\ & - \frac{1}{3\sqrt{6}} 0,2,3\rangle_x + \frac{1}{3\sqrt{6}}e^{\frac{i\pi}{3}} 0,2,5\rangle_x - \frac{1}{3\sqrt{6}} 0,3,4\rangle_x - \frac{1}{3\sqrt{6}} 0,3,5\rangle_x \\ & + \frac{1}{3\sqrt{6}}e^{\frac{i\pi}{3}} 0,4,5\rangle_x + \frac{1}{3\sqrt{6}}e^{\frac{i\pi}{3}} 1,2,3\rangle_x + \frac{1}{3\sqrt{6}}e^{-\frac{i\pi}{3}} 1,2,4\rangle_x + \frac{1}{3\sqrt{6}}e^{\frac{i\pi}{3}} 1,2,5\rangle_x \\ & + \frac{1}{3\sqrt{6}}e^{-\frac{i\pi}{3}} 1,3,4\rangle_x + \frac{1}{3\sqrt{6}}e^{-\frac{i\pi}{3}} 1,4,5\rangle_x - \frac{1}{3\sqrt{6}} 2,3,4\rangle_x + \frac{1}{3\sqrt{6}}e^{\frac{i\pi}{3}} 2,3,5\rangle_x \\ & + \frac{1}{3\sqrt{6}}e^{\frac{i\pi}{3}} 2,4,5\rangle_x + \frac{1}{3\sqrt{6}}e^{-\frac{i\pi}{3}} 3,4,5\rangle_x \end{aligned} $
$\hat{K} 0,1,2\rangle_p$	$ \begin{aligned} & - \frac{1}{6\sqrt{6}} 0,1,2\rangle_x + \frac{1}{3\sqrt{6}}e^{-\frac{i\pi}{3}} 0,1,3\rangle_x + \frac{1}{3\sqrt{6}}e^{-\frac{2i\pi}{3}} 0,1,4\rangle_x + \frac{1}{6\sqrt{6}} 0,1,5\rangle_x \\ & + \frac{1}{3\sqrt{6}}e^{-\frac{2i\pi}{3}} 0,2,3\rangle_x - \frac{1}{2\sqrt{6}} 0,2,4\rangle_x + \frac{1}{3\sqrt{6}}e^{\frac{2i\pi}{3}} 0,2,5\rangle_x + \frac{1}{3\sqrt{6}}e^{\frac{2i\pi}{3}} 0,3,4\rangle_x \\ & + \frac{1}{3\sqrt{6}}e^{\frac{i\pi}{3}} 0,3,5\rangle_x - \frac{1}{6\sqrt{6}} 0,4,5\rangle_x + \frac{1}{6\sqrt{6}} 1,2,3\rangle_x + \frac{1}{3\sqrt{6}}e^{\frac{2i\pi}{3}} 1,2,4\rangle_x \\ & + \frac{1}{3\sqrt{6}}e^{\frac{i\pi}{3}} 1,2,5\rangle_x + \frac{1}{3\sqrt{6}}e^{\frac{i\pi}{3}} 1,3,4\rangle_x + \frac{1}{2\sqrt{6}} 1,3,5\rangle_x + \frac{1}{3\sqrt{6}}e^{-\frac{i\pi}{3}} 1,4,5\rangle_x \\ & - \frac{1}{6\sqrt{6}} 2,3,4\rangle_x + \frac{1}{3\sqrt{6}}e^{-\frac{i\pi}{3}} 2,3,5\rangle_x + \frac{1}{3\sqrt{6}}e^{-\frac{2i\pi}{3}} 2,4,5\rangle_x + \frac{1}{6\sqrt{6}} 3,4,5\rangle_x \end{aligned} $

Table C.6: Expansion of $\hat{K}$ -projected momentum-space states in terms of position-space states of $N = 3$ hardcore bosons on $d = 6$ sites (continued).

Setting	State(s)	$\vec{\lambda}$
(N=2,d=3)	$\hat{K} 0,0\rangle_p, \hat{K} 1,1\rangle_p, \hat{K} 2,2\rangle_p$	$\{4/3, 1/3, 1/3\}$
(N=2,d=3)	$\hat{K} 0,1\rangle_p, \hat{K} 1,2\rangle_p, \hat{K} 0,2\rangle_p$	$\{4/3, 1/3, 1/3\}$
(N=2,d=4)	$\hat{K} 0,0\rangle_p, \hat{K} 1,1\rangle_p, \hat{K} 2,2\rangle_p, \hat{K} 3,3\rangle_p$	$\{3/2, 1/6, 1/6, 1/6\}$
(N=2,d=4)	$\hat{K} 0,1\rangle_p, \hat{K} 0,2\rangle_p, \hat{K} 0,3\rangle_p$	$\{1/2, 1/2, 1/2, 1/2\}$
(N=2,d=4)	$\hat{K} 1,2\rangle_p, \hat{K} 1,3\rangle_p, \hat{K} 2,3\rangle_p$	$\{1/2, 1/2, 1/2, 1/2\}$
(N=3,d=4)	$\hat{K} 0,0,0\rangle_p, \hat{K} 1,1,1\rangle_p, \hat{K} 2,2,2\rangle_p, \hat{K} 3,3,3\rangle_p$	$\{3/2, 1/2, 1/2, 1/2\}$
(N=3,d=4)	$\hat{K} 0,1,2\rangle_p, \hat{K} 0,2,3\rangle_p, \hat{K} 1,2,3\rangle_p, \hat{K} 0,1,3\rangle_p$	$\{3/2, 1/2, 1/2, 1/2\}$
(N=3,d=5)	$\hat{K} 0,0,0\rangle_p, \hat{K} 1,1,1\rangle_p, \hat{K} 2,2,2\rangle_p$	$\{\frac{9}{5}, \frac{3}{10}, \frac{3}{10}, \frac{3}{10}, \frac{3}{10}\}$
(N=3,d=5)	$\hat{K} 3,3,3\rangle_p, \hat{K} 4,4,4\rangle_p$	$\{\frac{9}{5}, \frac{3}{10}, \frac{3}{10}, \frac{3}{10}, \frac{3}{10}\}$
(N=3,d=5)	$\hat{K} 0,1,2\rangle_p, \hat{K} 0,1,3\rangle_p, \hat{K} 0,1,4\rangle_p, \hat{K} 1,3,4\rangle_p$	$\{\frac{43}{35}, \frac{23}{35}, \frac{23}{35}, \frac{8}{35}, \frac{8}{35}\}$
(N=3,d=5)	$\hat{K} 0,1,1\rangle_p, \hat{K} 0,2,2\rangle_p, \hat{K} 0,3,3\rangle_p, \hat{K} 1,2,2\rangle_p$	$\{\frac{4}{5}, \frac{4}{5}, \frac{7}{15}, \frac{7}{15}, \frac{7}{15}\}$
(N=3,d=6)	$\hat{K} 0,0,0\rangle_p, \hat{K} 1,1,1\rangle_p, \hat{K} 2,2,2\rangle_p$	$\{2, \frac{1}{5}, \frac{1}{5}, \frac{1}{5}, \frac{1}{5}, \frac{1}{5}\}$
(N=3,d=6)	$\hat{K} 3,3,3\rangle_p, \hat{K} 4,4,4\rangle_p, \hat{K} 5,5,5\rangle_p$	$\{2, \frac{1}{5}, \frac{1}{5}, \frac{1}{5}, \frac{1}{5}, \frac{1}{5}\}$
(N=3,d=6)	$\hat{K} 0,1,2\rangle_p, \hat{K} 0,1,5\rangle_p, \hat{K} 0,4,5\rangle_p, \hat{K} 1,2,3\rangle_p$	$\{1, \frac{2}{3}, \frac{2}{3}, \frac{1}{3}, \frac{1}{3}, 0\}$
(N=3,d=6)	$\hat{K} 0,1,3\rangle_p, \hat{K} 0,1,4\rangle_p, \hat{K} 0,2,3\rangle_p, \hat{K} 0,3,5\rangle_p$	$\{\frac{2}{3}, \frac{2}{3}, \frac{2}{3}, \frac{2}{3}, \frac{1}{3}, 0\}$
(N=3,d=6)	$\hat{K} 0,2,4\rangle_p, \hat{K} 1,3,5\rangle_p$	$\{1, 1, 1, 0, 0, 0\}$
(N=3,d=6)	$\hat{K} 0,1,1\rangle_p, \hat{K} 0,2,2\rangle_p, \hat{K} 1,2,2\rangle_p, \hat{K} 1,4,4\rangle_p$	$\{1, \frac{1}{2}, \frac{1}{2}, \frac{1}{3}, \frac{1}{3}, \frac{1}{3}\}$

Table C.7: $\vec{\lambda}$ -vectors of hardcore-projected bosonic momentum-state permanents for various settings of particle numbers and numbers of lattice sites.

Appendix D

Constrained optimisation and the Karush-Kuhn-Tucker formalism

In this section, we will introduce the terminology of constrained optimisation and summarise key theorems of that discipline. The presentation will follow the textbooks of Nocedal and Wright [73] and Bertsekas [10]. Constrained optimisation considers the problem of finding the (global) minimum of a multivariate function $f : \mathbb{R}^n \rightarrow \mathbb{R}$ on a constrained domain $\Omega \subsetneq \mathbb{R}^n$:

$$\min_{\vec{x} \in \Omega} f(\vec{x}). \quad (\text{D.1})$$

Commonly, f is called the *objective* or *utility* function. Ω is called the *feasibility domain* and will be defined by a set of algebraic constraints:

$$c_i(\vec{x}) = 0 \quad \text{for } i \in \mathcal{E}; \quad c_i(\vec{x}) \geq 0 \quad \text{for } i \in \mathcal{I}, \quad (\text{D.2})$$

where $\mathcal{E}$ and $\mathcal{I}$ represent finite index sets of the families of *equality* and *inequality* constraints.¹ Consequently, Ω can be written as:

$$\Omega \equiv \{\vec{x} \in \mathbb{R}^n \mid c_i(\vec{x}) = 0, \ i \in \mathcal{E} \quad \wedge \quad c_i(\vec{x}) \geq 0, \ i \in \mathcal{I}\}. \quad (\text{D.3})$$

Henceforth, the objective and constraint functions f and c_i will be considered to be smooth, even though it is possible to weaken this condition and extend the theorems introduced below to more general types of functions.

Constraints on the domain imprint constraints on the related tangent bundle $T\Omega$: A non-zero vector $\vec{d}$ will be called a *feasible direction* at point $\vec{x}_0$ if there exists a (piecewise smooth) curve $\vec{\gamma} : \mathbb{R} \supset [a, b] \rightarrow \Omega$ such that for $\vec{x}_0 = \vec{\gamma}(t_0)$ with $t_0 \in [a, b]$

¹Note that equality constraints are treated separately for practical reasons in later applications. Each equality constraint $c_i = 0$ could in principle be replaced by two inequality constraints $c_{i_1} = c_i \geq 0$ and $-c_{i_2} = -c_i \geq 0$.

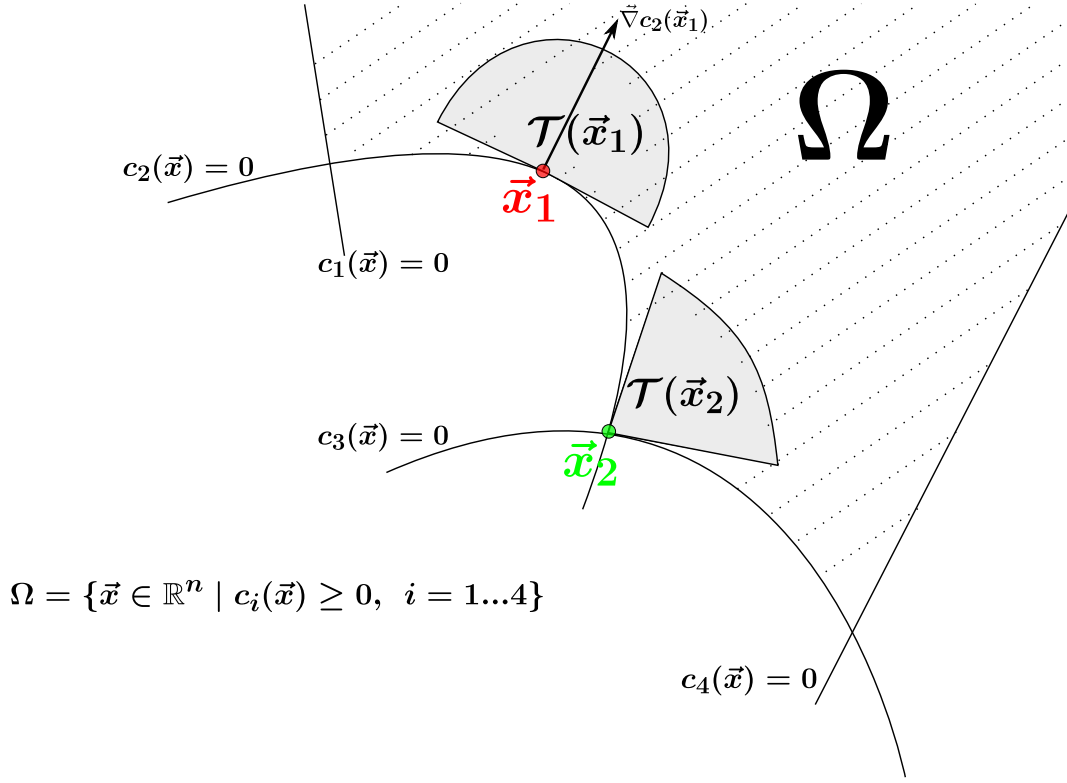


Figure D.1: Feasibility domain Ω and inequality constraints $c_i(\vec{x}) \geq 0$. For two points $\vec{x}_1$ and $\vec{x}_2$, the respective sets of unit length vectors in the tangent cones $\mathcal{T}(\vec{x}_1)$ and $\mathcal{T}(\vec{x}_2)$ are represented by light-grey fields. The gradient of c_2 at $\vec{x}_1$ is indicated by a black arrow. Whereas both constraints c_2 and c_3 are active in $\vec{x}_2$ (green point), only c_2 is active in $\vec{x}_1$ (red point).

the vector $\vec{d}$ is given by $\vec{d} = d\vec{\gamma}/dt|_{t_0}$. The set of all feasible directions at a point $\vec{x} \in \Omega$ forms the *tangent cone*:

$$\mathcal{T}(\vec{x}) \equiv \{\vec{d} \in \mathbb{R}^n; \quad \vec{d} \text{ is a feasible direction from } \vec{x}\}. \quad (\text{D.4})$$

At each point $\vec{x} \in \Omega$ the set of inequality constraints $\{c_i \geq 0\}_{i \in \mathcal{I}}$ decomposes into the set of *active* constraints

$$\{c_i \mid c_i(\vec{x}) = 0\} \equiv \{c_i\}_{i \in \mathcal{A}_{\vec{x}}} \quad (\text{D.5})$$

and the set of *inactive* constraints $\{c_i \mid c_i(\vec{x}) \neq 0\}$. Note that the index set of active constraints has been named as $\mathcal{A}_{\vec{x}} \subseteq \mathcal{I}$ and that every equality constraint may also be regarded active. By definition, however, $\mathcal{A}_{\vec{x}}$ does not comprise $\mathcal{E}$. A graphical illustration of these geometrical concepts is shown in Figure D.1.

This sketch further suggests that the angle between the gradient of a constraint function at a point where it is active and any feasible direction $\vec{d}$ is less or equal $\pi/2$, i.e. $\vec{\nabla} c \cdot \vec{d} \geq 0$.

More rigorously, we can start by looking at some equality constraint $c_{i_e}(\vec{x})_{i_e \in \mathcal{E}} = 0$. For any curve $\vec{\gamma}(t)_{t \in [a,b]} \in \Omega$ the function $\tilde{\gamma}(t) \equiv c_{i_e}(\vec{\gamma}(t))$ is obviously null on $t \in [a, b]$; taking the derivative therefore immediately implies:

$$\vec{\nabla} c_{i_e}(\vec{x}) \cdot \vec{d} = 0 \quad \forall \vec{d} \in \mathcal{T}(\vec{x}) \text{ and } i_e \in \mathcal{E}, \quad (\text{D.6})$$

i.e. the gradient of any equality constraint is always orthogonal to all feasible directions at any feasible point. This can be generalised to active inequality constraints. Let $c_i(\vec{x})_{i \in \mathcal{I}} \geq 0$ be an inequality constraint and $\vec{x}'$ a feasible point where it is active, i.e. $c_i(\vec{x}') = 0$. For any feasible direction $\vec{d}$ from $\vec{x}'$ a parallel infinitesimal direction $\vec{\Delta} \sim \vec{d}$ can be chosen such that $c_i(\vec{x}' + \vec{\Delta}) \geq 0$ since $\vec{x}' + \vec{\Delta} \in \Omega$. A look at the Taylor expansion of c_i around $\vec{x}'$ therefore establishes that

$$\vec{\nabla} c_i(\vec{x}') \cdot \vec{d} \geq 0 \quad \forall \vec{d} \in \mathcal{T}(\vec{x}') \text{ and } i \in \mathcal{A}_{\vec{x}'}. \quad (\text{D.7})$$

Together, Equations (D.6) and (D.7) motivate the definition of the set of *first order feasible directions*:

$$\mathcal{F}(\vec{x}) \equiv \{\vec{d} \in \mathbb{R}^n \mid \vec{\nabla} c_{i_e}(\vec{x}) \cdot \vec{d} = 0 \quad \forall i_e \in \mathcal{E} \text{ and } \vec{\nabla} c_i(\vec{x}') \cdot \vec{d} \geq 0 \quad \forall i \in \mathcal{A}_{\vec{x}}\}. \quad (\text{D.8})$$

Due to (D.6) and (D.7), it immediately follows that $\mathcal{T}(\vec{x}) \subseteq \mathcal{F}(\vec{x})$. The equality however, does not generally hold. The tangent cone is a purely geometrically defined object. By contrast, the form of $\mathcal{F}$ relies on the choice of constraint functions, which for some fixed domain Ω is not unique.² A feasible point $\vec{x}$ shall be called *quasi-regular* if $\mathcal{T}(\vec{x}) = \mathcal{F}(\vec{x})$.

In order to determine conditions on those points $\vec{x}$ that globally or locally minimise the objective function f , one has to consider the gradient field $\vec{\nabla} f$. For unconstrained optimisation, $\vec{\nabla} f(\vec{x}) = 0$ constitutes a necessary condition. In the case of a constrained domain Ω (D.3), conditions for the minima of the objective function may be determined by observing that a point $\vec{x} \in \Omega$ cannot be a minimum if there exists a feasible direction $\vec{d}$ at $\vec{x}$ for which f descends, i.e. $\vec{\nabla} f \cdot \vec{d} < 0$. Therefore, a necessary condition for a minimum is given by $\vec{\nabla} f(\vec{x}) \cdot \vec{d} \geq 0$ for all feasible directions $\vec{d} \in \mathcal{T}(\vec{x})$. The Karush-Kuhn-Tucker theorem³ makes use of this idea and

²The lack of uniqueness can be well demonstrated by considering a feasible domain defined by a single inequality constraint $c(\vec{x}) \geq 0$. The same geometrical set of points can also be defined by the alternative constraint function $\tilde{c}(\vec{x}) = c(\vec{x})^2 \geq 0$. Both constraint functions, however, have generally different gradients.

³Although already derived by William Karush in his master thesis in 1939 (see [49, 47]), the theorem initially remained unrecognised and was firstly attributed to Harald Kuhn and Albert Tucker in 1951 [57]. More recent literature however, acknowledges all three authors. The Karush-Kuhn-Tucker theorem therefore does not provide an extension of the formerly known Kuhn-Tucker theorem.

provides necessary conditions for the minimising points of a multivariate function on a constraint domain:

Theorem 5 (Karush-Kuhn-Tucker)

Let $\vec{x}'$ be a local minimum of the objective function $f : \mathbb{R}^n \rightarrow \mathbb{R}$ in the constrained domain Ω (D.3). Assume further that f and the constraint functions c_i are continuously differentiable. If $\vec{x}'$ is a quasi-regular point, then there exist Lagrangian multipliers λ_j , $j \in \mathcal{E}$ and μ_i , $i \in \mathcal{I}$ such that:

$$\vec{\nabla} f|_{\vec{x}'} = \sum_{j \in \mathcal{E}} \lambda_j \vec{\nabla} c_j|_{\vec{x}'} + \sum_{j \in \mathcal{I}} \mu_j \vec{\nabla} c_j|_{\vec{x}'}, \quad (\text{D.9a})$$

$$c_j(\vec{x}') = 0 \quad \forall j \in \mathcal{E}, \quad (\text{D.9b})$$

$$c_i(\vec{x}') \geq 0 \quad \forall i \in \mathcal{I}, \quad (\text{D.9c})$$

$$\mu_i \geq 0 \quad \forall i \in \mathcal{I} \quad \text{and} \quad (\text{D.9d})$$

$$\mu_i c_i(\vec{x}') = 0 \quad \forall i \in \mathcal{I}. \quad (\text{D.9e})$$

Solutions to these equations are called Karush-Kuhn-Tucker points (KKT-points). Equation (D.9e) implies that the Lagrange multiplier of an inactive constraint has to be strictly positive. The theorem states necessary conditions on minimising points. In order to determine the global minimum, one firstly has to check quasi-regularity of the domain followed by a case-by-case analysis of the activity or inactivity of the inequality constraints $c_i \geq 0$, $i \in \mathcal{I}$. Evaluating the objective function at the resulting KKT-points and taking the minimum value will then yield the global minimum.

A full proof of the Karush-Kuhn-Tucker theorem may be found in Refs. [73, 10].

Sufficient conditions for Quasi-Regularity

The application of the Karush-Kuhn-Tucker theorem requires Quasi-regularity of the inequality constraints. It therefore proves helpful to identify conditions for Quasi-regularity of a point $\vec{x}^* \in \Omega$, i.e. $\mathcal{T}(\vec{x}^*) = \mathcal{F}(\vec{x}^*)$. In the following, we list two important conditions. The proofs may be found in the cited literature.

1. Affine conditions (AC): Every point of the feasibility domain Ω is quasi-regular if all equality and inequality constraint functions (D.2) are linear functions [10].
2. Linear independence constraint qualifications (LICQ): A point $\vec{x} \in \Omega$ is quasi-regular if the gradients of the active inequality constraint and equality constraint functions are linearly independent in $\vec{x}$ [73].

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