On the Problem of Representability and the Bogoliubov–Hartree–Fock Theory

Hans Konrad Knörr

Dissertation

Technische Universität Braunschweig

On the Problem of Representability and the Bogoliubov–Hartree–Fock Theory

Von der
Carl–Friedrich–Gauß–Fakultät
der Technischen Universität Carolo–Wilhelmina zu Braunschweig

zur Erlangung des Grades eines
Doktors der Naturwissenschaften (Dr. rer. nat.)

genehmigte Dissertation
(kumulative Dissertation)

von
Hans Konrad Knörr
geboren am 31.08.1982
in Ansbach

Eingereicht am 26. Juli 2013
Disputation am 22. November 2013
1. Referent: Prof. Dr. Volker Bach
2. Referent: Prof. Dr. Heinz Siedentop

(2013)

Colophon

On the Problem of Representability and the Bogoliubov–Hartree–Fock Theory

A dissertation by Hans Konrad Knörr. Written under the supervision of Volker Bach at the Institut für Analysis und Algebra, Carl–Friedrich–Gauß–Fakultät, Technische Universität Braunschweig.

Contains one figure (created with the vector graphics editor Xfig).

Typeset using LaTeX and the memoir document class. The text is set with the Palatino font at 10.0/12.0pt, and the Pazo Math fonts are used for mathematical formulae.

Among the packages used are the AMS packages `amsfonts`, `amsmath`, `amssymb`, as well as `babel`, `dsfont`, `fontenc`, `graphicx`, `hyperref`, `inputenc`, `mathpazo`, `mathtools`, `ntheorem`, `soul`, and `url`. Questions and comments are welcome, and can be sent to the author by emailing `hansknoerr@gmx.de`.

Preface

The present thesis discusses questions which originate from quantum chemistry. The results also hold for more general physical systems consisting of fermions or bosons. It is a cumulative dissertation and its main body are the following three papers: "Generalized One-Particle Density Matrices and Quasifree States" [BBKM13], "Fermion Correlation Inequalities derived from G- and P-Conditions" [BKM12], and "Representability Conditions by Grassmann Integration" [BKM13]. Following this preface we outline the results of this thesis in an English and in a German summary.

* * *

Many people have, directly or indirectly, contributed to the success of my PhD thesis and I am grateful to all of them. Mentioning all of them would, however, go beyond the scope of this preface. Therefore I only have the possibility to thank those individually which had the greatest influence in my PhD project.

First of all, I wish to express my deep gratitude to my supervisor Volker Bach for the opportunity to work on this interesting project. His great expertise in many-body quantum mechanics, but also in other fields of mathematical physics, was a great benefit for me and this work.

Moreover, I am indebted to Edmund Menge for his friendship and many fruitful discussions. Despite often appearing disagreements, these discussion were one of the driving forces for our joint work.

Furthermore, I am grateful to Luigi Delle Site for his scientific support and interest in the PhD project.

A great help in writing this dissertation has been the use of a LaTeX template which is based on Matthias Westrich's and Rasmus Villamoes' PhD theses and the proofreading of parts of the manuscript by S. Breteaux, E. Menge, and T. Mühlenbruch. This work was supported in part by the Max Planck Graduate Center in Mainz.

Lastly, I am deeply grateful to my parents and my family for their support and encouragement during my PhD studies.

Hans Konrad Knörr
Ansbach, July 2013

Summary

The general topic of this thesis is an approximation of the ground state energy for many-particle quantum systems. In particular the Bogoliubov–Hartree–Fock theory and the representability of one- and two-particle density matrices are studied. After an introductory chapter we specify some basic notation of many-body quantum mechanics in Chapter 2. The Chapters 3 to 5 comprehend the papers [BBKM13], [BKM12], and [BKM13].

In Chapter 3 we consider boson, as well as fermion systems. We first tackle the question of representability for bosons, i.e., the question which conditions a one- and a two-particle operator must satisfy to ensure that they are the one- and the two-particle density matrix of a state. For a particle number-conserving system, the representability conditions up to second order for bosons are well-known [GP64, GM04] and called admissibility, P-, and G-conditions. Since, however, most physical systems consisting of bosons are not particle number-conserving, we give an alternative for such systems: Generalizing the two-particle density matrix, we observe that the representability conditions up to second order hold if and only if this generalized two-particle density matrix is positive semi-definite and the one- and the two-particle density matrices fulfill trace class and symmetry conditions. Moreover, we study the Bogoliubov–Hartree–Fock energy of boson and fermion systems. We generalize Lieb's variational principle [Lie81] which in its original formulation holds for purely repulsive particle interactions for fermions only. Our second main result is the following: for bosons, as well as for fermions the infimum of the energy for a variation over pure quasifree states coincides with the one for a variation over all quasifree states under the assumption that the Hamiltonian is bounded below. In the last section of Chapter 3 we specify the relation between centered quasifree states and their corresponding generalized one-particle density matrix, which finds an application in the variational process in the Bogoliubov–Hartree–Fock theory. It is well-known that the generalized one-particle density matrix of a pure quasifree fermion state is a projection, and uniquely determines this pure quasifree state [BLS94, Sol07]. We show that for fermions only pure quasifree states have a generalized one-particle density matrix which is a projection, and a similar statement for bosons which is the third main result.

Chapter 4 is concerned with fermion representability conditions and a relation to the fermion correlation inequalities. After two introductory sections specifying the problem and notation, we derive the representability conditions up to second order for fermions. We explain that these basic conditions on the one- and two-particle density matrices, namely the admissibility and the G-, P-, and Q-conditions, arise from certain expectation values of polynomials of degree two in fermion creation and annihilation operators. Furthermore we verify that there are no further independent conditions that can be obtained that way. The main result proven in Chapter 4 is the theorem stating that the admissibility, and the G- and P-conditions imply the fermion correlation inequality which was used in [Bac92] to derive a lower bound to the ground state energy. This lower bound is equal to the Hartree–Fock energy minus an error term which is small in the limit of large particle numbers. Thus a similar lower bound can already been obtained if one just requires the representability conditions mentioned above.

In the last chapter we study representability conditions for fermions. There are several different versions of representability conditions, but to our knowledge all of them use the Fock representation of the canonical anticommutation relations. In Chapter 5 we reformulate the representability conditions up to third order using Grassmann integrals. While Grassmann integration is a very common method in quantum field theory, representability conditions from quantum chemistry have not been studied within this framework. This transcription in another mathematical language will hopefully yield new insights into the problem of representability. Ingredients for this transcription are the introduction of a positivity property for Grassmann variables and the definition of an analogue of a density matrix, called Grassmann density. We prove that a certain Grassmann integral of such positive Grassmann variables is non-negative as the fundamental theorem of this chapter. We show that the representability conditions up to third order are implied by this fundamental theorem. Finally we adopt the notion of quasifree density matrices for Grassmann densities, allowing for a future study of the Hartree–Fock theory within the Grassmann integration formalism.

Zusammenfassung

Den Hauptteil dieser Dissertation bilden drei Artikel zu Fragen, die ihren Ursprung in der Vielteilchen-Quantenmechanik haben. In den ersten beiden Kapiteln führen wir zu den behandelten Fragestellungen hin und den mathematischen Formalismus ein.

Kapitel 3 besteht aus dem Artikel „Generalized One-Particle Density Matrices and Quasifree States" [BBKM13], der zur Veröffentlichung eingereicht ist. Wir beschäftigen uns zunächst mit der Frage der Darstellbarkeit für Bosonen, d.h. welche Bedingungen an Ein- und Zweiteilchenoperatoren stellen sicher, daß diese die Ein- und Zweiteilchendichtematrizen eines Zustandes sind. Für teilchenzahlerhaltende bosonische Systeme wurden die Darstellbarkeitsbedingungen bis zur zweiten, aber auch höherer Ordnung bereits untersucht und werden Zulässigkeit und G- und P-Bedingung genannt [GP64, GM04]. Da aber die meisten aus Bosonen bestehenden physikalischen Systeme nicht teilchenzahlerhaltend sind, geben wir eine Alternative für diese Systeme: Nachdem wir eine Verallgemeinerung der Zweiteilchendichtematrix einführen, stellen wir fest, daß die Darstellbarkeitsbedingungen bis zur zweiten Ordnung genau dann gelten, wenn diese verallgemeinerte Zweiteilchendichtematrix positiv semidefinit ist und die Ein- und die Zweiteilchendichtematrix eine bestimmte Symmetriebedingung und Spurklassebedingungen erfüllen. Das zweite Resultat beschäftigt sich mit der Bogoliubov–Hartree–Fock–Energie eines bosonischen oder fermionischen Systems mit nach unten beschränktem Hamiltonian. Wir verallgemeinern das Liebsche Variationsprinzip [Lie81], welches in seiner ursprünglichen Formulierung für Fermionen mit rein repulsivem Wechselwirkungspotential gilt, auf diese Systeme. Genauer gesagt zeigen wir, daß für diese Systeme auch eine auf reine quasifreie Zustände eingeschränkte Variation die Bogoliubov–Hartree–Fock–Energie liefert. Schließlich untersuchen wir die Beziehung zwischen zentrierten quasifreien Zuständen und deren verallgemeinerten Einteilchendichtematrizen, was eine Anwendung im Variationsprozeß in der Bogoliubov–Hartree–Fock–Theorie finden kann. Es ist bekannt, daß die verallgemeinerte Einteilchendichtematrix eines reinen quasifreien Zustandes für Fermionen eine Projektion ist und eindeutig diesen reinen quasifreien Zustand bestimmt [BLS94, Sol07]. Wir zeigen als drittes Resultat dieses Kapitels, daß für Fermionen nur reine quasifreie Zustände verallgemeinerte Einteilchendichtematrizen haben, die eine Projektion sind, und eine analoge Aussage für Bosonen.

Das Kapitel 4 befaßt sich mit fermionischen Darstellbarkeitsbedingungen und deren Beziehung zu fermionischen Korrelationsungleichung-en. Es entspricht der Veröffentlichung „Fermion Correlation Inequalities Derived from G- and P-Conditions“ [BKM12]. Nach zwei einleitenden Abschnitten, in denen wir das Problem dar- und die Notation festlegen, leiten wir die Darstellbarkeitsbedingungen bis zur zweiten Ordnung für Fermionen her. Wir begründen, daß die Zulässigkeit und die G-, P- und Q-Bedingung von bestimmten Erwartungswerten von Polynomen zweiter Ordnung in fermionischen Erzeugungs- und Vernichtungsoperatoren abgeleitet werden können, und, daß es keine weiteren, davon unabhängigen Bedingungen gibt, die man auf diese Weise gewinnen kann. Das wichtigste Ergebnis dieses Kapitels ist allerdings, daß die Zulässigkeit und die G- und die P-Bedingung bereits die fermionische Korrelationsungleichung implizieren, die in [Bac92] benutzt wurde, um eine untere Schranke an die Grundzustandsenergie herzuleiten. Diese untere Schranke stimmt mit der Hartree–Fock–Energie minus eines Fehlertermes, der für große Teilchenzahlen klein ist, überein. Demzufolge gilt eine analoge untere Schranke an die Grundzustandsenergie bereits, wenn man nur die oben erwähnten Darstellbarkeitsbedingungen an die Ein- und Zweiteilchendichtematrix voraussetzt. Insbesondere wird die Q-Bedingung in der Herleitung der Ungleichung nicht benötigt.

Im letzten Kapitel verbleiben wir bei den Darstellbarkeitsbedingungen für Fermionen. Es gibt viele verschiedene Versionen dieser Darstellbarkeitsbedingungen, aber unseres Wissens benutzen diese die Fockdarstellung der kanonischen Antivertauschungsrelationen. Während Grassmannvariablen und die Grassmannintegration in der Quantenfeldtheorie eine große Rolle spielen, wurde die Frage der Darstellbarkeit aus der Quantenchemie noch nicht in diesem Rahmen untersucht. In Kapitel 5 formulieren wir die Darstellbarkeitsbedingungen bis zur dritten Ordnung unter Verwendung von Grassmannintegralen um. Unsere Hoffnung ist, daß die angegebene Übersetzung in diese mathematische Sprache neue Einsichten liefert. Zu diesem Zweck führen wir als wichtige Grundlagen eine Semidefinitheitseigenschaft für Grassmannvariablen und ein Grassmannanalogon zu den Dichtematrizen ein, welches wir als Grassmanndichte bezeichnen. Als wichtigste Aussage dieses Kapitels wird gezeigt, daß das Grassmannintegral solcher positiven Grassmannvariablen nichtnegativ ist. Im Anschluß werden die Darstellbarkeitsbedingungen bis zur dritten Ordnung daraus hergeleitet. Desweiteren wird zum Abschluß angegeben, wie der Begriff der Quasifreiheit auf Grassmanndichten übertragen werden kann, was eine zukünftige Untersuchung der Hartree–Fock–Theorie im Rahmen des Grassmannintegral-Formalismus ermöglichen soll. Eine Version dieses Kapitels ist als Artikel „Representability Conditions by Grassmann Integration“ [BKM13] zur Veröffentlichung eingereicht.

Contents

Chapter 1

Introduction

As the name implies, many-body quantum mechanics is a physical theory for quantum systems consisting of N particles where N is a possibly huge natural number. Of particular interest for these systems is the ground state energy, i.e., the lowest energy expectation value, and the corresponding ground state. Unfortunately this ground state and its energy cannot be computed exactly for most systems. Nevertheless there are methods to approximate the ground state energy, as well as the ground state, and to estimate the error of the approximation. Two of these methods are the subject matter of this thesis: the Bogoliubov–Hartree–Fock theory and a method related to the representability of reduced density matrices.

The first method is a generalization of the Hartree-Fock theory to systems where the number of particles can change in its time evolution. The Hartree–Fock theory yields an upper bound to the exact ground state energy and is based on the so-called variational principle. From its development in the 1930's it took growing processing powers of computers, until it was commonly used to study the energetic properties of electron systems like atoms and molecules. For fermionic matter it is still one of the standard approximation methods in quantum chemistry to estimate the ground state and the ground state energy. The Bogoliubov–Hartree–Fock theory, or also called generalized Hartree–Fock theory, was developed in the last 20 years. A good account of this theory can be found, e.g., in [BLS94] for fermions and in [Sol06, Sol07] for bosons. The number of particles is not fixed in the Bogoliubov–Hartree–Fock theory, but it is itself a result obtained in the computation of the lowest energy expectation value, the Bogoliubov–Hartree–Fock energy, and the corresponding state. The Bogoliubov–Hartree–Fock energy is an upper bound to the ground state energy of the system.

The other method to tackle the ground state energy is connected to the problem of representability. Here the reduction of an N-particle wave function to a one- and a two-particle density matrix is crucial. These one- and two-particle density matrices are operators on the one- and two-particle Hilbert spaces. Given a Hamiltonian of a system with no higher interactions than pair interactions, they completely determine the energy of the system in the state described by the N-particle wave function. Thus the degrees of freedom are reduced in the computation of individual energy expectation values. It is, however, a complicated and still unsolved task to characterize the set of all pairs of one- and two-particle density matrices. This is referred to as the "problem of representability". Starting in the 1950's, representability conditions have been derived obtaining sets of necessary conditions on the reduced density matrices [Löw55, Col63, GP64, Erd78a, Erd78b]. After some quiet time, the research in this area has intensified in the last decade and yielded new insights and results. Recently an algorithm has been published to gradually derive representability conditions of higher orders for fermion systems [Maz12a, Maz12b]. Nevertheless a complete set of conditions cannot be computed in practice. Sufficient sets of conditions have, however, been used to produce lower bounds to the ground state energy, see, e.g., [CLS06].

Before we give an overview of the results of this thesis, we present some of the physical models for which the results are valid. We henceforth use those units in which the reduced Planck's constant $\hbar$, Coulomb's constant K_{e}, and the elementary charge e are $+1$, and the mass of the mainly considered particle is $1/2$. Furthermore we only consider nonrelativistic models. Therefore we neglect relativistic effects in our analysis.

1 Physical Models

The physical systems of interest are diverse and we only state a few of them explicitly. However, they all have in common that they can be described by an semi-bounded Hamiltonian $\mathbb{H}$ on the respective Fock space $\mathcal{F}^{\pm} \equiv \mathcal{F}^{\pm}[\mathfrak{h}]$ over a separable Hilbert space $\mathfrak{h}$. Here $\mathcal{F}^{\pm}$ denotes either the Fock space $\mathcal{F}^{+}$ of symmetric wave functions representing boson systems or the Fock space $\mathcal{F}^{-}$ of antisymmetric wave functions describing fermions. This Fock representation corresponds to the grand canonical ensemble known from statistical mechanics. Furthermore interaction potentials which link more than two particles are not considered.

1.1 Atoms and Molecules

The first model we want to mention is one for atoms and molecules. The Hamiltonian of an atom or a molecule with N electrons and K nuclei with charges $\underline{Z} := (Z_1, \ldots, Z_K)$ and positions $\underline{R} := (R_1, \ldots, R_K)$ ($K = 1$ for atoms) is given by

$$H^{(N)}(\underline{Z}, \underline{R}) := \sum_{n=1}^{N} \left(-\Delta_{x_n} - \sum_{k=1}^{K} \frac{Z_k}{|x_n - R_k|} \right) + \sum_{1 \leq n < m \leq N} \frac{1}{|x_n - x_m|}$$

in first order of the Born–Oppenheimer approximation. In the Born–Oppenheimer approximation the positions of the nuclei are assumed to be fixed at positions $R_1, \ldots, R_K$ which is justified by the relatively large mass of the nuclei compared to the small mass of the electron. For each $n = 1, \ldots, N$, x_n denotes the position of the n-th electron. The negative Laplacian $-\Delta_{x_n}$ represents the kinetic energy of the n-th electron. The attraction between the n-th electron and the k-th nucleus is given by the Coulomb potential $-\frac{Z_k}{|x_n - R_k|}$ and the last sum in the Hamiltonian denotes the mutual repulsion of the N electrons, again by a Coulomb potential. For more details and the second quantization $\mathbb{H}$ of this Hamiltonian see Chapter 4, Sections 1 and 2.4.

1.2 Bose Gas and Bosonic Atoms

We present only three prominent models of a Bose gas in three spatial dimensions. For an overview of results for the Bose gas see, e.g., [RSSS12, Chapter2]. For a more detailed survey of results for the Bose gas we refer to [LSSY05, ZB01].

The Bose gas is a sample of bosons which are confined in a box $\Lambda_L \subseteq \mathbb{R}^3$ of length L or trapped by an external potential. The simplest case is the ideal Bose gas confined to a box of length L with suitable boundary conditions. Here the bosons do not interact and there is no external potential. The N-particle Hamiltonian of this system is the sum of the kinetic energies of the bosons:

$$H_N := -\sum_{n=1}^{N} \Delta_{x_n}.$$

Assume that the density of the Bose gas is fixed to a value ρ. The system shows Bose–Einstein condensation for a proper thermodynamic limit $L \to \infty$, which keeps the density ρ fixed. Bose–Einstein condensation is a phenomenon first experimentally discovered in 1908 by K. Onnes in liquid helium. If the temperature of the system is below a critical value $T_c(\rho)$, two different aggregate states appear: part of the bosons are still in the gas phase, but a macroscopic part is in the ground state, forming a condensate. The one-particle density matrix defined in the next section can be used to quantify the macroscopic part. One criterion for Bose–Einstein condensation is for instance that one eigenvalue of the one-particle density matrix has to be of order N. This implies that most of the particles are in the same state.

A step higher in complexity is a Bose gas with a particle interaction v and a low density ρ, again in a box of length L. The particle interaction is assumed to be suitably short range, radially symmetric, and repulsive. We denote the scattering length of the interaction potential by a. The N-particle Hamiltonian of this so-called dilute Bose gas is

$$H_N := -\sum_{n=1}^{N} \Delta_{x_n} + \sum_{1 \le n < m \le N} v(|x_n - x_m|).$$

Let $\epsilon(\rho) := \lim_{L\to\infty} \frac{E_{\mathrm{gs}}(N,L)}{N}$ where $E_{\mathrm{gs}}(N,L)$ is the ground state energy and $\rho = \frac{N}{L^3}$ is kept fixed. Then $\epsilon(\rho) \approx 4\pi\rho a$ for small ρa^3 [LY98] and Bose–Einstein condensation is not needed to explain the ground state energy.

Finally we mention a boson system which is related to the atoms discussed in the previous section. It is called bosonic atom and is obtained from the usual atoms by assuming the electrons were bosons. The Hamiltonian on the symmetric N-particle Fock space is given by

$$H^{(N)}(Z,R) := \sum_{n=1}^{N} \left(-\Delta_{x_n} - \frac{Z}{|x_n - R|} \right) + \sum_{1 \le n < m \le N} \frac{1}{|x_n - x_m|}$$

where Z is the charge of the nucleus which is fixed at position R. The bosonic atom as well as bosonic molecules have been studied in [Bac91] to determine the ionization energy using the Hartree approximation. In [Nam11] the bosonic atom is discussed within the Bogoliubov theory, i.e., the variation is over non-particle number-conserving quasifree states which are not necessarily centered, i.e., expectation values of single creation or annihilation operators can be non-zero. In this context it is noteworthy that atoms, molecules etc., would not be stable if electrons were bosons. The instability of bosonic matter was proven by Dyson in 1967 [Dys67]. Later the asymptotics of the ground state energy in the limit of large particle numbers were determined more precisely. A lower bound for the asymptotics of the ground state energy was proven by Lieb and Solovej [LS04] and an upper bound by Solovej [Sol06]. These two bounds, derived for a more general model called two-component charged Bose gas, confirmed Dyson's conjectured asymptotic behaviour. The proof of stability of atoms and molecules with fermionic electrons was first given by Dyson and Lenard in 1967/68 [DL67, LD68]. A later proof by Lieb and Thirring in 1975 [LT75] had a great impact on mathematical physics. An outline of results for bosonic as well as fermionic matter with respect to stability is given in [LS10] and, more condensed, in [RSSS12, Chapter 3].

As stated before, this is not a complete list of the physical models covered in this thesis. It should only give an impression of the models the following results might be valid for.

2 Outline and Results

The basic notation and mathematical concepts are discussed in Chapter 2 in more detail. The subsequent Chapters 3 to 5 consist of the papers [BBKM13], [BKM12], and [BKM13]. Therefore the respective necessary notation is (re-) introduced at the beginning of each chapter.

The physical quantity, which this thesis is mostly concerned with, is the ground state energy, i.e., the infimum of the spectrum of a given Hamiltonian $\mathbb{H}$:

$$E_{\text{gs}} := \inf \{\sigma(\mathbb{H})\} .$$

An early attempt to approach the ground state energy of a Hamiltonian is the Rayleigh–Ritz variational principle

$$E_{\text{gs}} = \inf \left\{ \langle \Phi, \mathbb{H}\Phi \rangle_{\mathcal{F}} \,\middle|\, \Phi \in \mathcal{F}^{\pm},\ \|\Phi\|^2 = 1 \right\} . \tag{1.1}$$

The Rayleigh–Ritz principle originates from the study of vibrating plates and was first elaborated more than one hundred years ago [Ray78, Rit09a, Rit09b]. In principle, the normalized wave function $\Phi \in \mathcal{F}^{\pm}$ contains all information about the system that is in the pure state ω_Φ given by $\omega_\Phi(\,\cdot\,) := \langle \Phi, (\,\cdot\,)\Phi\rangle$. Consequently $\omega_\Phi(\mathbb{H}) = \langle \Phi, \mathbb{H}\Phi\rangle$ is the energy of the system if it is in the state ω_Φ. The notion of states can be extended from pure states described by a wave function to a suitable set of functionals ω which assign a real number to the Hamiltonian (and other selfadjoint operators called observables). The states form a convex set with the pure states as extreme elements. We remark that the state, as well as the wave function and the Hamiltonian, are, however, abstract objects and cannot be measured directly in physical experiments. The measurable quantities are expectation values as for example the energy expectation value $\omega(\mathbb{H})$. Using the general notion of states, the Rayleigh–Ritz principle can be rewritten as

$$E_{\mathrm{gs}} = \inf\left\{\omega(\mathbb{H}) \,\middle|\, \omega \text{ is a state}\right\}. \tag{1.2}$$

The number of degrees of freedom in this variation is, however, too large and for most systems it is an impossible task to determine the ground state that way. Thus, it seems promising to reduce the degrees of freedom. To this end the one- (1-pdm) and two-particle density matrices (2-pdm) $\gamma_\omega \in \mathcal{L}^1(\mathfrak{h})$ and $\Gamma_\omega \in \mathcal{L}^1(\mathfrak{h} \times \mathfrak{h})$ of a state ω are defined by their matrix elements

$$\langle f, \gamma_\omega g\rangle := \omega(a^*(g)a(f)) \text{ and} \tag{1.3}$$

$$\langle f_1 \otimes f_2, \Gamma_\omega(g_1 \otimes g_2)\rangle := \omega(a^*(g_1)a^*(g_2)a(f_2)a(f_2)) \tag{1.4}$$

for $f, g, f_1, f_2, g_1, g_2 \in \mathfrak{h}$, respectively. Here a^* and a denote the usual creation and annihilation operators on $\mathcal{F}^+$ for bosons and on $\mathcal{F}^-$ for fermions. Furthermore the energy functional $\mathcal{E}$, given by

$$\mathcal{E}(\gamma_\omega, \Gamma_\omega) := \omega(\mathbb{H}),$$

often has a less complicated structure than $\omega(\mathbb{H})$ with the full state and Hamiltonian. Then the variation (1.2) reads

$$E_{\mathrm{gs}} = \inf\left\{\mathcal{E}(\gamma, \Gamma) \,\middle|\, (\gamma, \Gamma) \text{ is representable}\right\}.$$

Here the notion of "representability" appears for the first time:

Definition 1.1. We say that a pair (γ, Γ) of a one- and a two-particle operator is representable if there is a state ω that has γ as its one- and Γ as its two-particle density matrix.

Given this definition, the question (or problem) of representability arises: How can one verify that given one- and two-particle operators are in fact the one- and two-particle density matrices of an unknown state? First of all, we cannot give the answer to this question (at least no feasible answer). Nevertheless this question is the starting point for approaching the ground state energy using representability conditions. Despite the fact that this set of conditions on the one- and two-particle operators is not complete, it is quite powerful to estimate the ground state energy.

2.1 Generalized One-Particle Density Matrices and Quasifree States

In Chapter 3 we consider boson, as well as fermion systems. After introducing the basic notation we tackle the question of representability for bosons in Section 3. For a particle number-conserving system the representability conditions up to second order for bosons are well-known [GP64, GM04] and called admissibility, P-, and G-conditions. Except for trace conditions of the one- and two-particle density matrices they arise from the positivity of expectation values of the form

$$\omega\left(\mathcal{P}^{*}\mathcal{P}\right) \tag{1.5}$$

where ω is a state and $\mathcal{P}$ a polynomial of degree two in boson creation and annihilation operators. As, however, most physical systems consisting of bosons are not particle number-conserving, we give an alternative for such systems. To this end we define a generalization of the two-particle density matrix. For this generalized two-particle density matrix we have:

Theorem 1.2. *The representability conditions up to second order hold if and only if the generalized two-particle density matrix is positive semi-definite, the pair (γ, Γ) of the one- and two-particle density matrices is in $\mathcal{L}^1(\mathfrak{h}) \times \mathcal{L}^1(\mathfrak{h}\otimes\mathfrak{h})$ with $\mathrm{tr}_{\mathfrak{h}}(\gamma) < \infty$, and the two-particle density matrix is symmetric, i.e., $\Gamma\,\mathrm{Ex} = \mathrm{Ex}\,\Gamma = \Gamma$ with the exchange operator $\mathrm{Ex}: \mathfrak{h}\otimes\mathfrak{h} \to \mathfrak{h}\otimes\mathfrak{h}$, $f\otimes g \mapsto g\otimes f$.*

This theorem can be used as a starting point of the future study of bosonic representability conditions.

In Section 4 we turn toward the Bogoliubov–Hartree–Fock energy

$$E_{\mathrm{BHF}} := \inf\left\{\omega(\mathbb{H}) \,\middle|\, \omega \text{ is a quasifree state}\right\}$$

with a Hamiltonian $\mathbb{H}$ on the boson or fermion Fock space $\mathcal{F}^{\pm}[\mathfrak{h}]$. The Bogoliubov–Hartree–Fock energy is an upper bound to the ground state energy since the variation is restricted compared to the one in (1.2). For particle number-conserving systems the Bogoliubov–Hartree–Fock energy matches the Hartree–Fock energy. In its original formulation, Lieb's variational principle for the Hartree–Fock energy

$$E_{\mathrm{hf}} := \inf\left\{\omega(\mathbb{H}) \,\middle|\, \omega \text{ is a particle number-conserving pure quasifree state}\right\}$$

states that in fact

$$E_{\mathrm{hf}} = \inf\left\{\omega(\mathbb{H}) \,\middle|\, \omega \text{ is a particle number-conserving quasifree state}\right\}$$

for purely repulsive particle interactions for fermions [Lie81]. We present a generalization of Lieb's variational principle. More precisely we show the following theorem for bosons, as well as for fermions:

Theorem 1.3. *Let $\mathbb{H}$ be a Hamiltonian that is bounded below. Then*

$$E_{\mathrm{BHF}} = \inf\left\{\omega(\mathbb{H}) \,\middle|\, \omega \textit{ is a pure quasifree state}\right\}.$$

It is remarkable that we do not need particle number-conservation or repulsiveness of the interaction potential. Recently a version of this theorem for the so-called fiber Hamiltonian in the Pauli–Fierz model has been shown in [BBT13].

In the last section of Chapter 3 the relation between a centered quasifree state ω and its corresponding generalized one-particle density matrix $\widetilde{\gamma}_\omega$ is specified. The generalized one-particle density matrix is an operator on $\mathfrak{h} \oplus \mathfrak{h}$ and can be written as

$$\widetilde{\gamma}_\omega = \begin{pmatrix} \gamma_\omega & \alpha_\omega \\ \overline{\alpha}_\omega & \mathbb{1}_{\mathfrak{h}} \pm \overline{\gamma}_\omega \end{pmatrix}$$

where $\gamma_\omega = \gamma_\omega^*$ is the usual one-particle density matrix, $\alpha_\omega = \pm\alpha_\omega^T$, and the plus-sign holds for bosons and the minus-sign for fermions. It is well-known [BLS94] that the generalized one-particle density matrix $\widetilde{\gamma}$ of a pure quasifree fermion state is a projection,

$$\widetilde{\gamma}^2 = \widetilde{\gamma} = \widetilde{\gamma}^*, \tag{1.6}$$

and that two distinct pure quasifree states cannot have the same generalized one-particle density matrix. For bosons a similar statement holds true for centered pure quasifree states and their generalized one-particle density matrix $\widetilde{\gamma}$ which satisfies

$$\widetilde{\gamma}\mathcal{S}\widetilde{\gamma} = -\widetilde{\gamma} \tag{1.7}$$

where $\mathcal{S} := \begin{pmatrix} \mathbb{1}_{\mathfrak{h}} & 0 \\ 0 & -\mathbb{1}_{\mathfrak{h}} \end{pmatrix} \in \mathcal{B}(\mathfrak{h} \oplus \mathfrak{h})$, [Sol07, Nam11]. As the third result of this chapter we show the following:

Theorem 1.4. *The following statements are equivalent:*

(i) The centered state ω is pure and quasifree.

(ii) The generalized one-particle density matrix $\widetilde{\gamma}_\omega$ of the state ω satisfies (1.6) for fermions, (1.7) for bosons, and $\mathrm{tr}_{\mathfrak{h}}(\gamma_\omega) < \infty$.

Therefore the relation between centered pure quasifree states and their generalized one-particle density matrix is unique.

Interesting properties of two objects are examined in the appendix: a representation of the generalized two-particle density matrix as a 7×7-matrix and an algorithm to simplify certain polynomials of degree two in boson creation and annihilation operators are given.

2.2 Fermion Correlation Inequalities Derived from G- and P-Conditions

After considering both quantum particle types in the previous chapters, we now restrict our attention to fermion systems. The physical models mainly considered in Chapter 4 are atoms and molecules in first order of the Born-Oppenheimer approximation, i.e., a system of Z electrons interacting via a Coulomb potential and moving in the Coulomb field of the fixed nuclei. We study the ground state energy of this system and an approximation. To this end we observe that the representability conditions up to second order on the one- and two-particle density matrices arise from certain expectation values of the form (1.5):

Theorem 1.5. *Let ρ be a (not necessarily positive) trace class operator that is normalized, $\mathrm{tr}_{\mathcal{F}^-}(\rho) = 1$, particle number-conserving, $\widehat{\mathbb{N}}\rho = \rho\widehat{\mathbb{N}}$, and satisfies $\mathrm{tr}_{\mathcal{F}^-}(\rho\widehat{\mathbb{N}}^2) < \infty$. Denote by γ_ρ and Γ_ρ the one- and two-particle operators defined as in (1.3) and (1.4) neglecting that ρ is not necessarily a density matrix. Then the following statements are equivalent:*

(i) If $\mathcal{P}_r \in \mathcal{B}(\mathcal{F}^-)$ is a polynomial in creation and annihilation operators of degree $r \leq 2$, then $\mathrm{tr}_{\mathcal{F}^-}(\rho\mathcal{P}_r^*\mathcal{P}_r) \geq 0$.

(ii) The pair $(\gamma_\rho, \Gamma_\rho)$ is admissible and fulfills the G-, P- and Q-conditions.

Generally the representability conditions are conditions on the pair (γ, Γ) of a one- and a two-particle operator. These conditions ensure that γ and Γ are the one- and two-particle density matrices of a density matrix (or equivalently a state). The basic conditions, as well as conditions of higher order have been studied in quantum chemistry, e.g., in [Col63, GP64, GM04, Maz12a].

In [Bac92] the fermion correlation inequality

$$\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left((X \otimes X)\Gamma^{(T)}\right) \geq -\mathrm{tr}_{\mathfrak{h}}(X\gamma) \min\left\{1, c\sqrt{\mathrm{tr}_{\mathfrak{h}}(X(\gamma - \gamma^2))}\right\} \tag{1.8}$$

has been proven where c is a numerical constant, X an orthogonal projection, $\Gamma^{(T)} := \Gamma - (\mathbb{1}_{\mathfrak{h}\otimes\mathfrak{h}} - \mathrm{Ex})(\gamma \otimes \gamma)$ the truncated two-particle density matrix, and γ and Γ the one- and two-particle density matrices. Furthermore, this inequality was used to derive a lower bound to the ground state energy. This lower bound is the Hartree–Fock energy minus an error that is small in the limit of large particle numbers. For neutral atoms the obtained asymptotic behaviour reads

$$E_{\mathrm{gs}} \geq E_{\mathrm{hf}} - \mathcal{O}\left(Z^{\frac{5}{3}-\epsilon}\right)$$

for some $\epsilon > 0$ and large atomic number Z. Note that E_{gs} and E_{hf} also depend on Z.

In Section 4 we show that the fermion correlation inequality (with a different constant than in [Bac92]) is already implied only assuming that (γ, Γ) fulfills some necessary representability conditions. More precisely, considering only the admissibility condition, the P-condition on Γ, i.e.,

$$\Gamma \geq 0,$$

and the G-condition,

$$\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left((A \otimes A)(\Gamma + \mathrm{Ex}(\gamma \otimes \mathbb{1}_{\mathfrak{h}}))\right) \geq |\mathrm{tr}_{\mathfrak{h}}(A\gamma)|^2$$

for any $A \in \mathcal{B}(\mathfrak{h})$, we show the main result of Chapter 4:

Theorem 1.6. *Let X be an orthogonal projection, γ and Γ a one- and a two-particle operator and $\Gamma^{(T)} := \Gamma - (\mathbb{1}_{\mathfrak{h}\otimes\mathfrak{h}} - \mathrm{Ex})(\gamma \otimes \gamma)$. If (γ, Γ) obeys the admissibility, and the G- and P-conditions, the fermion correlation inequality (1.8) with a slightly larger numerical constant than in [Bac92] holds.*

Therefore, the last theorem together with the calculations in [Bac92] yields that the lower bound "Hartree–Fock energy minus error" is already implied if we only assume the one- and two-particle density matrices to satisfy the representability conditions mentioned in the previous theorem.

There are further questions that arise at this point and are subject to future studies. On the one hand, one direction is an improvement of the estimate by considering more representability conditions. On the other hand, it is not clear that all conditions, used here to prove the fermion correlation inequality, are necessary and maybe the assumptions in Theorem 1.6 can be relaxed.

2.3 Representability Conditions by Grassmann Integration

Our focus remains on fermion representability conditions. There are several different versions of representability conditions, but to our knowledge the representability conditions have not been studied in the context of Grassmann integrals. The formalism using Grassmann variables and integration has proven its value in quantum field theory [Sal98, FKT02]. In Chapter 5 we reformulate representability conditions up to third order.

Let M be a finite index set and $\mathcal{H}$ an $|M|$-dimensional Hilbert space. The Grassmann algebra $\mathcal{G}_M$ is generated by the set $\{\overline{\psi}_i, \psi_i\}_{i\in M}$. These generators fulfill the anticommutation relations

$$\overline{\psi}_i\psi_j + \psi_j\overline{\psi}_i = \overline{\psi}_i\overline{\psi}_j + \overline{\psi}_j\overline{\psi}_i = \psi_i\psi_j + \psi_j\psi_i = 0$$

for any $i, j \in M$. Furthermore, a linear mapping between the bounded operators on the fermion Fock space $\wedge\mathcal{H}$ and the Grassmann algebra is defined. Then $\{\psi_i\}_{i\in M}$ can be considered as the orthonormal basis of the underlying, finite dimensional Hilbert space $\mathcal{H}$.

There are two important ingredients which introduce a notion of positivity and are given in Section 4. We define the (modified) Grassmann integral $\int \mathcal{D}(\overline{\Psi}, \Psi)$ as a linear functional $\mathcal{G}_M \to \mathbb{C}$ and the star product "$\mu \star \eta$" between any two Grassmann variables $\mu, \eta \in \mathcal{G}_M$. This star product induces a structure similar to the CAR for fermion creation and annihilation operators. After discussing some properties of the star product and the Grassmann integral, we define a positivity property for Grassmann variables as the first ingredient:

A Grassmann variable $\mu \in \mathcal{G}_M$ is called positive semi-definite, abbreviated by $\mu \geq 0$, if there is an $\eta \in \mathcal{G}_M$ such that $\mu = \eta^* \star \eta$.

Finally we can show as the second ingredient:

Theorem 1.7. *For any positive semi-definite $\mu \in \mathcal{G}_M$ we have*

$$(-1)^{|M|} \int \mathcal{D}(\overline{\Psi}, \Psi)\, \mu \geq 0.$$

In Section 5 we tackle the problem of representability by Grassmann integration. To this end we define a Grassmann analogue of a density matrix:

A Grassmann density is a positive semi-definite Grassmann variable $\varkappa$ which is normalized, i.e., $\int \mathcal{D}(\overline{\Psi},\Psi)\,\varkappa = 1$.

With this Grassmann density the one- and two-particle density matrices $\gamma_\varkappa$ and $\Gamma_\varkappa$ can be defined by

$$\langle \psi_k, \gamma_\varkappa \psi_l \rangle_{\mathcal{H}} := \int \mathcal{D}(\overline{\Psi},\Psi)\,\varkappa \star \overline{\psi}_l \star \psi_k,$$

$$\langle \psi_m \otimes \psi_n, \Gamma_\varkappa (\psi_l \otimes \psi_k) \rangle_{\mathcal{H}\otimes\mathcal{H}} := \int \mathcal{D}\left(\overline{\Psi},\Psi\right)\ \varkappa \star \overline{\psi}_k \star \overline{\psi}_l \star \psi_m \star \psi_n,$$

where $\{\psi_k\}_{k\in M}$ is an ONB of the underlying Hilbert space $\mathcal{H}$.

Then the representability conditions up to second order can be obtained using the previous theorem:

Theorem 1.8. *Let $\varkappa \in \mathcal{G}_M$ be a Grassmann density. Then the following statements are equivalent:*

(i) The pair $(\gamma_\varkappa, \Gamma_\varkappa)$ fulfills $0 \le \gamma_\varkappa \le \mathbb{1}_{\mathcal{H}}$ and the G-,P-, and Q-conditions.

(ii) $\int \mathcal{D}(\overline{\Psi},\Psi)\,\varkappa \star \mu \ge 0$ for any $\mu \in \mathcal{G}_M$ which is at most quartic in the generators of the Grassmann algebra $\mathcal{G}_M$.

Furthermore, we present a derivation of two further conditions that are representability conditions of third order. These conditions are called T_1-condition and generalized T_2-condition and obtained considering

$$\int \mathcal{D}(\overline{\Psi},\Psi)\varkappa \star (\tau^* \star \tau + \tau \star \tau^*) \ge 0$$

for certain $\tau \in \mathcal{G}_M$ which are cubic in the generators of $\mathcal{G}_M$.

Finally we adopt the notion of quasifree states to this formalism in Section 6. As for usual density matrices we can assign a Grassmann state $\langle\cdot\rangle_\varkappa : \mathcal{G}_M \to \mathbb{C}$ to each Grassmann density $\varkappa \in \mathcal{G}_M$ by

$$\langle \mu \rangle_\varkappa := \int \mathcal{D}(\overline{\Psi},\Psi)\,\varkappa \star \mu$$

for every $\mu \in \mathcal{G}_M$. We call this Grassmann state, as well as its corresponding Grassmann density, quasifree if it fulfills Wick's Theorem in a version for Grassmann variables. Adapting methods from [BLS94], we can show that quasifree Grassmann densities are of a specific form:

Theorem 1.9. *The Grassmann state given by*

$$\varkappa = \frac{1}{Z}\left(\Theta_0 \star \left[\left(\mathrm{e}^{-q_{i_1}} - 1\right)\overline{\psi}_{i_1}\psi_{i_1} + 1\right] \star \cdots \star \left[\left(\mathrm{e}^{-q_{i_m}} - 1\right)\overline{\psi}_{i_m}\psi_{i_m} + 1\right]\right)$$

is quasifree. $\{i_1,\ldots,i_m\} \subseteq M$, $q_{i_1},\ldots,q_{i_m} \in \mathbb{R}$, and $\Theta_0 \in \mathcal{G}_M$ are determined by the corresponding generalized one-particle density matrix $\widetilde{\gamma}_\varkappa = \begin{pmatrix} \gamma_\varkappa & 0 \\ 0 & \mathbb{1}_{\mathcal{H}} - \overline{\gamma}_\varkappa \end{pmatrix}$ and $1/Z$ is a normalization factor.

This allows for a investigation of the Hartree–Fock theory for fermions by means of Grassmann variables and integrals.

Starting from the notions of positivity and Grassmann densities elaborated in Chapter 5, a more detailed study of the representability of one- and two-particle density matrices within the framework of Grassmann integration will hopefully yield new insights. It may also result in a new, more practical characterization of quasifree Grassmann densities and consequently of the Hartree–Fock energy and the corresponding state.

CHAPTER 2

Mathematical Framework

Let $\mathcal{H}$ denote a complex Hilbert space with the inner product $\langle \cdot, \cdot \rangle_{\mathcal{H}} : \mathcal{H} \times \mathcal{H} \to \mathbb{C}$. An element $f \in \mathcal{H}$ of the Hilbert space is called *wave function*. For the inner product we choose the convention that it is antilinear in the first and linear in the second argument:

$$\langle \eta f_1 + f_2, g_1 \rangle_{\mathcal{H}} = \overline{\eta} \langle f_1, g_1 \rangle_{\mathcal{H}} + \langle f_2, g_1 \rangle_{\mathcal{H}},$$
$$\langle f_1, \eta g_1 + g_2 \rangle_{\mathcal{H}} = \eta \langle f_1, g_1 \rangle_{\mathcal{H}} + \langle f_1, g_2 \rangle_{\mathcal{H}}$$

for any $f_1, f_2, g_1, g_2 \in \mathcal{H}$ and any $\eta \in \mathbb{C}$. The norm induced by the inner product is given by

$$\|f\|_{\mathcal{H}} := \sqrt{\langle f, f \rangle_{\mathcal{H}}}$$

for any wave function f and turns $(\mathcal{H}, \|\cdot\|_{\mathcal{H}})$ into a Banach space. We call the Hilbert space $\mathcal{H}$ *separable* if there is a countable subset which is dense in $\mathcal{H}$. Then we can choose an orthonormal basis (ONB) $\{\varphi_k\}_{k \in \mathcal{M}}$ where $\langle \varphi_k, \varphi_l \rangle = \delta_{ij}$ and $\mathcal{M} \subseteq \mathbb{N}$ with $|\mathcal{M}| = \dim(\mathcal{H})$.
In the following we always presume that the Hilbert space $\mathcal{H}$ is separable with $\dim(\mathcal{H}) = \infty$, and $\mathcal{M} = \mathbb{N}$. E.g., for many physical systems in a d-dimensional space, this Hilbert space is chosen to be $L^2(\mathbb{R}^d; \mathbb{C})$, the vector space of all square-integrable functions, with the inner product $\langle f, g \rangle_{L^2} := \int_{\mathbb{R}^d} \mathrm{d}x \, \overline{f}(x) g(x)$ where $\overline{f}$ denotes the complex conjugate of the wave function $f \in L^2(\mathbb{R}^d; \mathbb{C})$.

A map $A : \mathcal{D}(A) \to \mathcal{H}_2$ satisfying $A(\mu f + g) = \mu A f + A g$ for any $\mu \in \mathbb{C}$ and any $f, g \in \mathcal{D}(A)$ is called a *linear operator* where $\mathcal{D}(A) \subseteq \mathcal{H}_1$ is the domain of the operator A and $\mathcal{H}_1$ and $\mathcal{H}_2$ two (not necessarily different) Hilbert spaces. In the following we only deal with linear operators and, if we speak of operators, we always assume them to be linear.
An operator A is *bounded* if it satisfies

$$\|A\|_{\mathrm{op}} := \sup \left\{ \|Af\|_{\mathcal{H}} \,\middle|\, f \in \mathcal{D}(A), \ \|f\|_{\mathcal{H}} = 1 \right\} < \infty$$

where $\|\cdot\|_{\mathrm{op}}$ is called operator norm. The set of all bounded operators on $\mathcal{H}$ is denoted by $\mathcal{B}(\mathcal{H})$. A selfadjoint operator A is *positive semi-definite*, abbreviated by $A \geq 0$, if

$$\langle f, Af \rangle_{\mathcal{H}} \geq 0$$

for any $f \in \mathcal{D}(A) \subset \mathcal{H}$. A is called *positive definite* if the inequality is strict, and *negative (semi-) definite* if $-A$ is positive (semi-) definite. Furthermore, an operator A is bounded above by another operator B, denoted by $A \leq B$, if $B - A$ is positive semi-definite. We call an operator A on $\mathcal{H}$ *trace class*, or shortly $A \in \mathcal{L}^1(\mathcal{H})$, if

$$\mathrm{tr}_{\mathcal{H}}(|A|) < \infty$$

where the *absolute value* of an operator is given by $|A| := \sqrt{A^*A}$. In particular, all trace class operators are bounded. The subset of all positive semi-definite trace class operators on $\mathcal{H}$ is denoted by $\mathcal{L}^1_+(\mathcal{H})$. The *Hilbert–Schmidt operators* are those operators A on $\mathcal{H}$, which satisfy

$$\mathrm{tr}_{\mathcal{H}}(A^*A) < \infty,$$

and the set of all Hilbert–Schmidt operators is denoted by $\mathcal{L}^2(\mathcal{H})$.

For any vector space $\mathcal{K}$ we denote the dual space, i.e., the set of all linear functionals $\mathcal{K} \to \mathbb{C}$, by $\mathcal{K}^*$. For a Hilbert space $\mathcal{H}$ any element of the dual space $\mathcal{H}^*$ can be expressed by f^* with $f \in \mathcal{H}$ where $f^*g := \langle f, g \rangle_{\mathfrak{h}}$ for every $g \in \mathcal{H}$.

Now let $\mathfrak{h}$ be a complex separable Hilbert space which we henceforth call the *one-particle Hilbert space*. For any $N \in \mathbb{N}$ the *N-particle Hilbert space* which represents a physical system consisting of N indistinguishable particles is given as the N-fold tensor product of copies of the one-particle Hilbert space, i.e.,

$$\mathfrak{h}^{\otimes N} := \bigotimes^N \mathfrak{h}.$$

The inner product $\langle \cdot, \cdot \rangle_{\mathfrak{h}^{\otimes N}} : \mathfrak{h}^{\otimes N} \times \mathfrak{h}^{\otimes N} \to \mathbb{C}$ is defined by

$$\langle f_1 \otimes \cdots \otimes f_N, g_1 \otimes \cdots \otimes g_N \rangle_{\mathfrak{h}^{\otimes N}} := \prod_{k=1}^{N} \langle f_k, g_k \rangle_{\mathfrak{h}}$$

for any $f_1, \ldots, f_N, g_1, \ldots, g_N \in \mathfrak{h}$. However, not every element of the N-particle Hilbert space can be written as such a tensor product of one-particle wave functions. Nevertheless, every N-particle wave function is at least the limit of a sequence of (finite) linear combinations of such tensor products. Thus, by linearity the definition of the inner product extends to all N-particle wave functions, as well.

If the number of particles is not conserved by the dynamics of the system, a common method to tackle such physical systems is the so-called *second quantization*. There the *Fock space* $\mathcal{F}$ is considered. It is defined as the direct sum of all N-particle Hilbert spaces,

$$\mathcal{F} \equiv \mathcal{F}[\mathfrak{h}] := \bigoplus_{N=0}^{\infty} \mathfrak{h}^{\otimes N}.$$

Here, by convention $\mathfrak{h}^{\otimes 0} := \mathbb{C}$ with the inner product given by $\langle \mu, \nu \rangle_{\mathfrak{h}^{\otimes 0}} := \overline{\mu}\nu$ for any $\mu, \nu \in \mathfrak{h}^{\otimes 0}$. Every element $\Psi \in \mathcal{F}$ can be written as a sequence of N-particle wave functions $f^{(N)} \in \mathfrak{h}^{\otimes N}$:

$$\Psi = (f_N)_{N=0}^{\infty}.$$

With the inner product $\langle \cdot, \cdot \rangle_{\mathcal{F}} : \mathcal{F} \times \mathcal{F} \to \mathbb{C}$ defined by

$$\langle \Psi, \Phi \rangle_{\mathcal{F}} := \sum_{N=0}^{\infty} \langle f_N, g_N \rangle_{\mathfrak{h}^{\otimes N}}$$

for any $\Psi \equiv (f_N)_{N=0}^{\infty}$ and $\Phi \equiv (g_N)_{N=0}^{\infty} \in \mathcal{F}$ the Fock space is a Hilbert space. As an important reference vector of the Fock space we introduce the *vacuum vector*

$$\Omega := (1, 0, 0, \dots) \in \mathcal{F}.$$

Since we only consider physical systems with at most pair interactions, i.e., no three-particle interactions or higher, it suffices to introduce the second quantization for one- and two-particle operators. A selfadjoint operator $h : \mathcal{D}(h) \to \mathfrak{h}$ with domain $\mathcal{D}(h) \subseteq \mathfrak{h}$ is extended to an operator

$$\mathbb{h} \equiv \mathrm{d}\Gamma(h) : \mathcal{D}(\mathbb{h}) \to \mathcal{F}$$

on the Fock space $\mathcal{F}$ with domain

$$\mathcal{D}(\mathbb{h}) := \left\{ (f_N)_{N=0}^{\infty} \in \mathcal{F} \middle| f_N \in \mathcal{D}(h^{(N)}) := (\mathcal{D}(h))^{\otimes N} \subseteq \mathfrak{h}^{\otimes N} \right\}$$

as follows. The operator h is first lifted to an operator $h^{(N)} := \sum_{k=1}^{N} h_k$ with $h_k := \left(\mathbb{1}_{\mathfrak{h}}^{\otimes k-1} \otimes h \otimes \mathbb{1}_{\mathfrak{h}}^{\otimes N-k} \right)$ on $\mathfrak{h}^{\otimes N}$ and then for any $\Psi \equiv (f_N)_{N=0}^{\infty} \in \mathcal{F}$, $f_N \in \mathcal{D}(h^{(N)})$, we define the N-th component of $\mathbb{h}$ for $N \in \mathbb{N} \cup \{0\}$ by

$$(\mathbb{h}\Psi)_N := h^{(N)} f_N.$$

Furthermore, the second quantization of a selfadjoint two-particle operator $V : \mathcal{D}(V) \to \mathfrak{h} \otimes \mathfrak{h}$, $\mathcal{D}(V) \subseteq \mathfrak{h} \otimes \mathfrak{h}$, that can be written as a (finite or infinite) linear combination of tensor products of the form $X \otimes X$, $X : \mathcal{B}(X) \to \mathfrak{h}$ with $\mathcal{B}(X) \subseteq \mathfrak{h}$, is extended in a similar way. An example of such a two-particle operator is the Coulomb interaction (cf. Lemma 4.8). For every $k, l \in \{1, \dots, N\}$ with $k \neq l$, $N \in \mathbb{N}$, and $N \geq 2$ we define the operator V_{kl} on $\mathfrak{h}^{\otimes N} = \mathfrak{h}_1 \otimes \mathfrak{h}_2 \otimes \cdots \otimes \mathfrak{h}_N$ with $\mathfrak{h}_i = \mathfrak{h}$, $i = 1, \dots, N$, as the operator which acts as the identity operator on all spaces except for $\mathfrak{h}_k$ and $\mathfrak{h}_l$ and links the spaces $\mathfrak{h}_k$ and $\mathfrak{h}_l$ with V. Then for every $N \in \mathbb{N}$ with $N \geq 2$ the second quantized operator $\mathbb{V} : \mathcal{D}(\mathbb{V}) \subseteq \mathcal{F} \to \mathcal{F}$ is given by

$$(\mathbb{V}\Psi)_N := V^{(N)} f_N$$

where $\Psi \equiv (f_N)_{N=0}^{\infty} \in \mathcal{D}(\mathbb{V})$, $f_N \in \mathfrak{h}^{\otimes N}$, $N \in \mathbb{N} \cup \{0\}$, and $V^{(N)} := \sum_{1 \leq k < l \leq N} V_{kl}$.

The second quantization $\mathbb{A}$ of a selfadjoint operator A is selfadjoint.

The *particle number operator* $\widehat{\mathbb{N}} : \mathcal{D}(\widehat{\mathbb{N}}) \to \mathcal{F}$ is defined as the second quantized identity operator $\mathbb{1}_{\mathfrak{h}}$, i.e.,

$$\widehat{\mathbb{N}} := \mathrm{d}\Gamma\left(\mathbb{1}_{\mathfrak{h}}\right),$$

with the domain

$$\mathcal{D}(\widehat{\mathbb{N}}) := \left\{ \Psi = (f_N)_{N=0}^{\infty} \in \mathcal{F} \,\middle|\, \sum_{N=0}^{\infty} (N+1)^2 \, \|f_N\|^2_{\mathfrak{h}^{\otimes N}} < \infty \right\}.$$

An easy computation shows that actually $\widehat{\mathbb{N}}\,(f_N)_{N=0}^{\infty} = (N f_N)_{N=0}^{\infty}$ for any $(f_N)_{N=0}^{\infty} \in \mathcal{F}$.

A more detailed description of the second quantization can be found in [BR79, BR81, Thi08].

1 Bosons

The *boson Fock space*, or symmetric Fock space, is the symmetric subspace of the Fock space $\mathcal{F}[\mathfrak{h}]$, i.e.,

$$\mathcal{F}^+ \equiv \mathcal{F}^+[\mathfrak{h}] := S \bigoplus_{N=0}^{\infty} \mathfrak{h}^{\otimes N}.$$

Here for any $N \in \mathbb{N}$ and any set $\{f_k\}_{k=1}^N \subset \mathfrak{h}$ the *symmetrization operator* $S \in \mathcal{B}(\mathcal{F})$ is defined by

$$S \left(\bigotimes_{k=1}^{N} f_k \right)_{N=0}^{\infty} := \left(\frac{1}{N!} \sum_{\pi \in \mathfrak{S}_N} \bigotimes_{k=1}^{N} f_{\pi(k)} \right)_{N=0}^{\infty},$$

where $\mathfrak{S}_N$ denotes the symmetric group with permutations π of N elements.

Definition 2.1. For any $f \in \mathfrak{h}$ the *boson creation and annihilation operators* are denoted by $a^*(f)$ and $a(f)$ with $a^*(f) = (a(f))^*$. Their domain is the dense subset

$$\mathcal{D}(\widehat{\mathbb{N}}^{\frac{1}{2}}) \cap \mathcal{F}^+ = \left\{ \Psi \equiv \left(f^{(N)}\right)_{N=0}^{\infty} \in \mathcal{F}^+ \,\middle|\, \sum_{N=0}^{\infty} (N+1) \left\| f^{(N)} \right\|^2 < \infty \right\}$$

of $\mathcal{F}^+$. They are completely characterized by the properties

$$a(f)\Omega = 0, \qquad a^*(f)\Omega = f,$$

and the *canonical commutation relations (CCR)*

$$[a^*(f), a^*(g)] = 0\,, \quad [a(f), a(g)] = 0\,, \quad \text{and} \quad [a(f), a^*(g)] = \langle f, g \rangle \, \mathbb{1}_{\mathcal{F}}$$

for any pair $(f, g) \in \mathfrak{h} \times \mathfrak{h}$ where $\mathbb{1}_{\mathcal{F}} \in \mathcal{B}(\mathcal{F})$ is the identity operator on the Fock space. $[A, B] := AB - BA$ denotes the commutator.

The creation operator $a^*(f)$ is linear in f while the annihilation operator $a(f)$ is antilinear. Since the particle number operator is unbounded and

$$\|a^*(f)\|_{\text{op}} \le \|f\|_{\mathfrak{h}} \left\| \left(\widehat{N} + \mathbb{1}_{\mathcal{F}}\right)^{\frac{1}{2}} \right\|_{\text{op}},$$

$$\|a(f)\|_{\text{op}} \le \|f\|_{\mathfrak{h}} \left\| \left(\widehat{N} + \mathbb{1}_{\mathcal{F}}\right)^{\frac{1}{2}} \right\|_{\text{op}},$$

the boson creation and annihilation operators are not bounded by $\mathbb{1}_{\mathcal{F}}$. We henceforth use the abbreviations $a_k^* \equiv a^*(\varphi_k)$ and $a_k \equiv a(\varphi_k)$ for any element of a given arbitrary orthonormal basis (ONB) $\{\varphi_k\}_{k=1}^{\infty}$ of $\mathfrak{h}$.

Let h be a one-particle operator on $\mathcal{D}(h) \subseteq \mathfrak{h}$. Given an arbitrary ONB $\{\varphi_k\}_{k=1}^{\infty}$ of $\mathcal{D}(h)$, the second quantization of h restricted to the boson Fock space, $\mathbb{h}\big|_{\mathcal{F}^+} := S\mathbb{h}S : \mathcal{D}(\mathbb{h}) \cap \mathcal{F}^+ \to \mathcal{F}^+$, can be expressed as

$$\mathbb{h}\big|_{\mathcal{F}^+} = \sum_{k,l=1}^{\infty} h_{kl}\, a_k^* a_l$$

as a quadratic form using the creation and annihilation operators. Here $h_{kl} := \langle \varphi_k, h\varphi_l \rangle_{\mathfrak{h}} \in \mathbb{C}$ for $k, l \in \mathbb{N}$. In particular, the particle number operator on $\mathcal{F}^+$ can be rewritten as

$$\widehat{\mathbb{N}} = \sum_{k=1}^{\infty} a_k^* a_k$$

for any ONB $\{\varphi_k\}_{k=1}^{\infty}$ of $\mathfrak{h}$. The second quantization $\mathbb{V}\big|_{\mathcal{F}^+} := S\mathbb{V}S : \mathcal{F}^+ \to \mathcal{F}^+$ of a two-particle operator $V : \mathfrak{h} \otimes \mathfrak{h} \to \mathfrak{h} \otimes \mathfrak{h}$ reads

$$\mathbb{V}\big|_{\mathcal{F}^+} = \sum_{k,l,m,n=1}^{\infty} V_{kl;mn}\, a_l^* a_k^* a_m a_n$$

where $V_{kl,mn} := \langle \varphi_k \otimes \varphi_l, V(\varphi_m \otimes \varphi_n) \rangle_{\mathfrak{h}\otimes\mathfrak{h}}$ for any $k, l, m, n \in \mathbb{N}$ and $\varphi_k \otimes \varphi_l \in \mathcal{D}(V)$ for any $k, l \in \mathbb{N}$.

1.1 The Weyl Operators and the CCR Algebra

Next we introduce the C^*-algebra of operators on the boson Fock space. Unlike the fermionic case the space generated by all boson creation and annihilation operators cannot be used. Therefore, we construct the so-called CCR algebra. For a detailed survey on the Weyl operators and the CCR algebra see, e.g., [BR81].

We define the *field operator* $\Phi(f) : \mathcal{F}^+ \to \mathcal{F}^+$ for every $f \in \mathfrak{h}$ by

$$\Phi(f) := \frac{1}{\sqrt{2}} \left(a^*(f) + a(f)\right). \tag{2.1}$$

The field operator is essentially selfadjoint on the boson Fock space and, therefore, its closure, which we also denote by $\Phi(f)$, is selfadjoint.

Definition 2.2. Let $f \in \mathfrak{h}$ and $\Phi(f)$ be the corresponding field operator defined in (2.1). We define the *Weyl operator* $\mathbb{W}(f) : \mathcal{F} \to \mathcal{F}$ for any $f \in \mathfrak{h}$ as the unitary map given by

$$\mathbb{W}(f) := \exp(\mathrm{i}\Phi(f)).$$

The Weyl operators satisfy $\mathbb{W}(f)^* = \mathbb{W}(-f)$ and the Weyl commutation relations

$$\mathbb{W}(f)\mathbb{W}(g) = \mathrm{e}^{-\frac{\mathrm{i}}{2}\operatorname{Im}\langle f,g\rangle_{\mathfrak{h}}}\mathbb{W}(f+g)$$

for any $f, g \in \mathfrak{h}$. The Weyl commutation relations completely determine the commutator of any two Weyl operators. Furthermore, we have $\mathbb{W}(0) = \mathbb{1}_{\mathcal{F}}$.

A given field operator $\Phi(f)$ with $f \in \mathfrak{h}$ is transformed by the Weyl operator $\mathbb{W}(g)$ with $g \in \mathfrak{h}$ as follows:

$$\mathbb{W}(g)\Phi(f)\mathbb{W}(g)^* = \Phi(f) - \operatorname{Im}\langle g, f\rangle_{\mathfrak{h}} \mathbb{1}_{\mathcal{F}}.$$

Thus, the transform of a creation operator $a^*(f)$ and an annihilation operator $a(f)$ can be specified for any $f \in \mathfrak{h}$. For an arbitrary $g \in \mathfrak{h}$ we obtain

$$\mathbb{W}_g a^*(f)\mathbb{W}_g^* = a^*(f) + \langle g, f\rangle_{\mathfrak{h}} \quad \text{and} \mathbb{W}_g a(f)\mathbb{W}_g^* = a(f) + \langle g, f\rangle_{\mathfrak{h}}$$

where $\mathbb{W}_g \equiv \mathbb{W}(\mathrm{i}\sqrt{2}g)$ is the so-called Weyl transformation.

Definition 2.3. The C^*-algebra $\mathcal{W}$ generated by $\{\mathbb{W}(f) | f \in \mathfrak{h}\}$ is called Weyl algebra or *CCR algebra*.

This algebra is unique up to $*$-automorphisms (Cf. Theorem 5.2.8. of [BR81]). We call the selfadjoint elements of the Weyl algebra *observables*. They represent physically measurable properties of the system like the energy or the positions of the particles.

1.2 States and Density Matrices

Complementarily to the observables the state comprehends all information contained in the physical system and determines all quantities we can measure.

Definition 2.4. A continuous linear functional $\omega \in \mathcal{W}^*$ on the Weyl algebra $\mathcal{W}$ is called a *state* if it is normalized and positive, i.e., if $\omega(\mathbb{1}_{\mathcal{F}}) = 1$ and $\omega(A) \geq 0$ for all positive semi-definite operators $A \in \mathcal{W}$.

For $A \in \mathcal{W}$ the complex number $\omega(A)$ is called expectation value of A. This expectation value of A is real and corresponds to the measured value for the quantity, which is represented by A, of the system in the state ω.

Since the creation and annihilation operators are not bounded by $\mathbb{1}_{\mathcal{F}}$ for bosons, their expectation values are not well-defined for all states. We restrict ourselves to a subset of states since we will consider also expectation values of creation and annihilation operators. To this end, let $\mathbb{W}(f)$ denote a Weyl operator for any $f \in \mathfrak{h}$. We assume that for the state ω the map

$$T_f : \mathbb{R} \to \mathbb{C},\ t \mapsto \omega\big(\mathbb{W}(tf)\big)$$

is four times continuously differentiable for all $f \in \mathfrak{h}$, shortly denoted by $T_f \in \mathcal{C}^4(\mathbb{R};\mathbb{C})$. Then we can state a definition of the expectation value of a single creation or annihilation operator and of the particle number operator. For instance, we have

$$\omega\big(\Phi(f)\big) := \frac{\mathrm{d}}{\mathrm{d}t}\,\omega\big(\mathbb{W}(tf)\big)\Big|_{t=0} < \infty$$

for any $f \in \mathfrak{h}$ and by linearity of ω we get

$$\omega(a(f)) = \frac{1}{\sqrt{2}}\left[\omega\big(\Phi(f)\big) + \mathrm{i}\omega\big(\Phi(\mathrm{i}f)\big)\right].$$

Analogously we obtain

$$\omega\big(a^*(f)\big), \quad \omega\big(e(f)\,e(g)\big), \quad \text{and} \quad \omega\big(e(f_1)\,e(f_2)\,e(g_2)\,e(g_1)\big)$$

for $f, g, f_1, f_2, g_1, g_2 \in \mathfrak{h}$ due to $T_f \in \mathcal{C}^4(\mathbb{R};\mathbb{C})$ where e denotes either the creation operator a^* or the annihilation operator a. In the state ω, for which $T_f \in \mathcal{C}(\mathbb{R};\mathbb{C})$, the expectation value for polynomials of degree four in creation and annihilation operators can be defined. We give a general polynomial of degree two as an example of such a polynomial:

Example. For any polynomial $\mathcal{P}_2$ of degree two there are an ONB $\{\varphi_k\}_{k=1}^{\infty}$ of $\mathfrak{h}$, an $N \in \mathbb{N}$, and coefficients $\alpha_{kl}, \beta_{kl}, \epsilon_{kl}, \zeta_k, \xi_k, \mu \in \mathbb{C},\ k, l \in \{1, \ldots, N\}$, such that

$$\mathcal{P}_2 = \sum_{k,l=1}^{N} \left[\alpha_{kl} a_k^* a_l + \beta_{kl} a_k^* a_l^* + \epsilon_{kl} a_k a_l\right] + \sum_{k=1}^{N} \left[\zeta_k a_k^* + \xi_k a_k\right] + \mu$$

We denote the extension of the CCR algebra to the polynomials of degree four by $\mathcal{A}$.

Definition 2.5. Given this new set $\mathcal{A}$, we define $\mathcal{A}^+ := \overline{\mathcal{A}}$ as its closure.

Given an ONB $\{\varphi_k\}_{k=1}^{\infty}$ of $\mathfrak{h}$, the polynomials $\widehat{\mathbb{N}}_N := \sum_{k=1}^{N} a_k^* a_k$ with $N \in \mathbb{N}$ form a monotonously increasing sequence which converges strongly to the particle number operator $\widehat{\mathbb{N}}$ on the domain

$$\mathcal{D}(\widehat{\mathbb{N}}) \cap \mathcal{F}^+ = \left\{ \Psi \equiv \left(f^{(N)}\right)_{N=0}^{\infty} \in \mathcal{F}^+ \,\middle|\, \sum_{N=0}^{\infty} (N+1)^2 \left\| f^{(N)} \right\|^2 < \infty \right\}.$$

Definition 2.6. We write $\omega \in \mathcal{Z}^+$ if ω satisfies the following conditions:

(i) ω is a state,

(ii) $T_f \in \mathcal{C}^4(\mathbb{R}; \mathbb{C})$, and

(iii) $\omega(\widehat{\mathbb{N}}^2) := \lim_{N\to\infty} \omega(\widehat{\mathbb{N}}_N^2) < \infty$.

The subset of all N-particle states is $\mathcal{Z}_N^+ := \left\{ \omega \in \mathcal{Z}^+ \middle| \, \omega(\widehat{\mathbb{N}}) = N \right\}$.

For any $\omega \in \mathcal{Z}^+$ the particle number expectation value is finite since by the Cauchy–Schwarz inequality

$$\omega(\widehat{\mathbb{N}}) \leq \sqrt{\omega(\widehat{\mathbb{N}}^2)} < \infty.$$

Definition 2.7. A state $\omega \in \mathcal{Z}^+$ is called *pure* if there is a $\Phi \in \mathcal{F}^+$ such that for any $A \in \mathcal{A}^+$

$$\omega(A) = \langle \Phi, A\Phi \rangle_{\mathcal{F}}.$$

Definition 2.8. We call a state $\omega \in \mathcal{Z}^+$ *centered* and write $\omega \in \mathcal{Z}_{\text{cen}}^+$ if

$$\omega(a^*(f)) = 0 \tag{2.2}$$

for any $f \in \mathfrak{h}$.

Any centered state satisfies $\omega(a(f)) = 0$ which follows from (2.2).

Definition 2.9. A state $\omega \in \mathcal{Z}^+$ is *quasifree*, shortly $\omega \in \mathcal{Z}_{\text{qf}}^+$, if there are a wave function $f_\omega \in \mathfrak{h}$ and a positive semi-definite operator h_ω on $\mathfrak{h}$ such that for every $f \in \mathfrak{h}$

$$\omega(\mathbb{W}_f) = \exp\left(2\mathrm{i} \, \langle f_\omega, f \rangle_{\mathfrak{h}} - \langle f, (\mathbb{1}_{\mathfrak{h}} + h_\omega) f \rangle_{\mathfrak{h}}\right)$$

where $\mathbb{W}_f$ denotes the Weyl transformation. The subset of pure quasifree states is denoted by $\mathcal{Z}_{\text{pqf}}^+$.

Remark 2.10. Note that the above definition of quasifreeness differs from the common ones, i.e., the property to satisfy Wick's Theorem in the version given below. Nevertheless, if we assume the quasifree state ω to be centered, it fulfills Wick's Theorem in a simplified version:

$$\begin{aligned} &\omega(e_1 e_2 \cdots e_{2N-1}) = 0 \quad \text{and} \\ &\omega(e_1 e_2 \cdots e_{2N}) = \sum_{\pi}{}' \, \omega(e_{\pi(1)} e_{\pi(2)}) \cdots \omega(e_{\pi(2N-1)} e_{\pi(2N)}) \end{aligned}$$

for every $N \in \mathbb{N}$. For every $i \in \{1, 2, \ldots, 2N\}$ e_i is either a creation or an annihilation operator. The prime at the summation symbol indicates that the sum is taken over all permutations $\pi \in \mathcal{S}_{2N}$ satisfying

$$\pi(1) < \pi(3) < \cdots < \pi(2N-1) \text{ and } \pi(2k-1) < \pi(2k)$$

for every $k \in \{1, 2, \ldots, N\}$.

Definition 2.11. We say that a state $\omega \in \mathcal{Z}^+$ is *coherent*, $\omega \in \mathcal{Z}^+_{\text{coh}}$, if there is a wave function $f \in \mathfrak{h}$ such that for all $A \in \mathcal{A}^+$

$$\omega(A) = \left\langle \Omega, \mathbb{W}_f^* A \mathbb{W}_f \Omega \right\rangle_{\mathcal{F}}.$$

Obviously any centered quasifree or pure quasifree state is quasifree. For bosons there are quasifree states that are not centered and ones that are not pure. Furthermore, the set of coherent states is a proper subset of the set of pure quasifree states.

The notion of states is a generalization of the density matrices used in quantum physics and chemistry.

Definition 2.12. A *density matrix* ρ is a positive semi-definite trace class operator with $\mathrm{tr}_{\mathcal{F}}(\rho) = 1$.

For any density matrix $\rho \in \mathcal{L}^1_+(\mathcal{F}^+)$ the map $\mathcal{A}^+ \to \mathbb{C}, A \mapsto \mathrm{tr}_{\mathcal{F}}(\rho A)$, defines a state (which is not necessarily in $\mathcal{Z}^+$). In particular, for every state $\omega \in \mathcal{Z}^+$ there is a density matrix ρ with $\mathrm{tr}(\rho A) = \omega(A)$ for all $A \in \mathcal{A}^+$.

1.3 One- and Two-Particle Density Matrices and Representability

Now we are prepared to define the one- and two-particle density matrices.

Definition 2.13. Let $\omega \in \mathcal{Z}^+$. The operator $\gamma_\omega : \mathfrak{h} \to \mathfrak{h}$ defined by

$$\langle f, \gamma_\omega g \rangle_{\mathfrak{h}} := \omega(a^*(g) a(f))$$

for every $f, g \in \mathfrak{h}$ is called *(boson) one-particle density matrix* (1-pdm).

The one-particle density matrix is a positive semi-definite trace class operator. Let $h : \mathcal{D}(h) \to \mathfrak{h}$ be an operator with domain $\mathcal{D}(h) \subseteq \mathfrak{h}$ and second quantization $\mathbb{h} : \mathcal{D}(\mathbb{h}) \cap \mathcal{F}^+ \to \mathcal{F}^+$. Then the expectation value of $\mathbb{h}$ in the state $\omega \in \mathcal{Z}^+$ can be rewritten as

$$\omega(\mathbb{h}) = \mathrm{tr}_{\mathfrak{h}}(h \gamma_\omega)$$

where $\gamma_\omega : \mathfrak{h} \to \mathfrak{h}$ is the 1-pdm of the state ω.

Definition 2.14. The *(boson) two-particle density matrix* (2-pdm) $\Gamma_\omega : \mathfrak{h} \otimes \mathfrak{h} \to \mathfrak{h} \otimes \mathfrak{h}$ of a state $\omega \in \mathcal{Z}^+$ is given by

$$\langle f_1 \otimes f_2, \Gamma_\omega (g_1 \otimes g_2) \rangle := \omega \left(a^*(g_2) a^*(g_1) a(f_1) a(f_2) \right)$$

for any $f_1, f_2, g_1, g_2 \in \mathfrak{h}$.

The two-particle density matrix is a positive definite trace class operator that is symmetric, i.e., $\Gamma_\omega (f \otimes g) = \Gamma_\omega (g \otimes f)$ for any $f, g \in \mathfrak{h}$. For a two-particle operator $V : \mathcal{D}(V) \to \mathfrak{h} \otimes \mathfrak{h}$, $\mathcal{D}(V) \subseteq \mathfrak{h} \otimes \mathfrak{h}$, with second quantization $\mathbb{V} : \mathcal{D}(\mathbb{V}) \cap \mathcal{F}^+ \to \mathcal{F}^+$ and any state $\omega \in \mathcal{Z}^+$ we obtain

$$\omega(\mathbb{V}) = \mathrm{tr}_{\mathfrak{h} \otimes \mathfrak{h}} (V \Gamma_\omega)$$

with the 2-pdm Γ_ω of ω.

Definition 2.15. We call a pair (γ, Γ) of bounded operators on $\mathfrak{h} \times (\mathfrak{h} \otimes \mathfrak{h})$ *admissible* if

(i) $\Gamma \in \mathcal{L}^1(\mathfrak{h} \otimes \mathfrak{h})$ is symmetric, i.e., $\mathrm{Ex}\Gamma = \Gamma\mathrm{Ex} = \Gamma$, and selfadjoint, and

(ii) $\gamma \in \mathcal{L}^1(\mathfrak{h})$ with $\mathrm{tr}_{\mathfrak{h}}(\gamma) = \omega\left(\widehat{\mathbb{N}}\right)$ is selfadjoint and positive semi-definite.

The *exchange operator* $\mathrm{Ex} : \mathfrak{h} \otimes \mathfrak{h} \to \mathfrak{h} \otimes \mathfrak{h}$ is defined by

$$\mathrm{Ex}(f \otimes g) := g \otimes f$$

for any $f, g \in \mathfrak{h}$.

Definition 2.16. We say that the pair (γ, Γ) of operators on $\mathfrak{h} \times (\mathfrak{h} \otimes \mathfrak{h})$ is *N-representable* if there is a state $\omega \in \mathcal{Z}_N^+$ with $\gamma_\omega = \gamma$ and $\Gamma_\omega = \Gamma$, and *representable* if there is a state $\omega \in \mathcal{Z}^+$ having γ as its 1-pdm and Γ as its 2-pdm. Necessary conditions on the pair (γ, Γ) to be representable are called *representability conditions*.

In particular, every representable pair (γ, Γ) is admissible.

1.4 Generalized One–Particle Density Matrices

A generalization of the Hartree–Fock theory for fermions was introduced 20 years ago by Bach, Lieb, and Solovej, [BLS94], by using a generalized one-particle density matrix. Later, Solovej extended this concept to boson systems [Sol06, Sol07] (see also [Nam11]). We provide a definition of the generalized 1-pdm.

Throughout this subsection we use a fixed, but arbitrary ONB of the one-particle Hilbert space $\mathfrak{h}$ which we denote by $\{\varphi_k\}_{k=1}^\infty$. We define the complex conjugate $\overline{f}$ of a function $f = \sum_{k=1}^\infty \mu_k \varphi_k \in \mathfrak{h}$ by $\overline{f} := \overline{\sum_{k=1}^\infty \overline{\mu}_k \varphi_k}$ and the complex conjugate $\overline{A}$ of an operator A by $\langle f, \overline{A} g\rangle_{\mathfrak{h}} := \overline{\left\langle \overline{f}, A\overline{g}\right\rangle_{\mathfrak{h}}}$. The transpose of an operator A is $A^T := \overline{A^*}$. Therefore, the following definitions depend on the choice of the ONB. We refer the reader to [Sol07] for a basis independent formulation.

Definition 2.17. Let $\omega \in \mathcal{Z}^+$. The corresponding *generalized one-particle density matrix* $\widetilde{\gamma}_\omega$ is the operator on $\mathfrak{h} \oplus \mathfrak{h}$ given by

$$\langle f_1 \oplus f_2, \widetilde{\gamma}_\omega (g_1 \oplus g_2)\rangle_{\mathfrak{h}\oplus\mathfrak{h}} := \omega\big([a^*(g_1) + a(\overline{g}_2)] \left[a(f_1) + a^*(\overline{f}_2)\right] \big)$$

for $f_1, f_2, g_1, g_2 \in \mathfrak{h}$.

Let $\omega \in \mathcal{Z}^+$. With

$$\alpha_\omega^* : \mathfrak{h} \to \mathfrak{h}\,,\ \langle f, \alpha_\omega^* g\rangle_{\mathfrak{h}} := \omega\big(a^*(g)\, a^*(\overline{f})\big),$$

the generalized 1-pdm can be written as a matrix with operator-valued entries:

$$\widetilde{\gamma}_\omega = \begin{pmatrix} \gamma_\omega & \alpha_\omega \\ \alpha_\omega^* & \mathbb{1}_\mathfrak{h} + \overline{\gamma}_\omega \end{pmatrix}.$$

An easy computation shows that α_ω is symmetric, i.e., $\alpha_\omega^T = \alpha_\omega$.

In Chapter 3 properties of this generalized 1-pdm are discussed, further generalizations of the one-, as well as the two-particle density matrix are introduced (Chapt. 3, Subsubsect. 2.1.4) and their relation to the bosonic representability problem is considered (Chapt. 3, Subsect. 3.2).

2 Fermions

The *fermion (or antisymmetric) Fock space* $\mathcal{F}^- \equiv \mathcal{F}^-[\mathfrak{h}] \equiv \bigwedge \mathfrak{h}$ is defined as the orthogonal sum

$$\mathcal{F}^-[\mathfrak{h}] := \bigoplus_{N=0}^{\infty} \mathfrak{h}^{\wedge N}$$

of the antisymmetrized N-particle Hilbert spaces

$$\mathfrak{h}^{\wedge N} := A_N \mathfrak{h}^{\otimes N}$$

which are antisymmetric tensor products of N copies of $\mathfrak{h}$ with $N \in \mathbb{N}$, and $\mathfrak{h}^{\wedge 0} := \mathbb{C}$. The *antisymmetrization operator* $A : \mathcal{F} \to \mathcal{F}^-$, $A := \bigoplus_{N=0}^{\infty} A_N$ with $A_N : \mathfrak{h}^{\otimes N} \to \mathfrak{h}^{\wedge N}$ is uniquely defined by

$$A_N \left(\bigotimes_{k=1}^{N} f_k \right) := \left(\frac{1}{N!} \sum_{\pi \in \mathfrak{S}_N} (-1)^\pi \bigotimes_{k=1}^{N} f_{\pi(k)} \right)_{N=0}^{\infty} =: \frac{1}{\sqrt{N!}} f_1 \wedge \cdots \wedge f_N,$$

for $f_1, \ldots, f_N \in \mathfrak{h}$, where $(-1)^\pi$ denotes the sign of the permutation $\pi \in \mathfrak{S}_N$.

Definition 2.18. The *fermion creation and annihilation operators* are bounded operators on the fermion Fock space $\mathcal{F}^-$, which we denote by $c^*(f)$ and $c(f)$, respectively, for any $f \in \mathfrak{h}$, and are completely characterized by the properties

$$c(f)\Omega = 0\,, \quad c^*(f)\Omega = f,$$

and the *canonical anticommutation relations* (CAR)

$$\{c^*(f), c^*(g)\} = 0, \ \{c(f), c(g)\} = 0, \text{ and } \{c(f), c^*(g)\} = \langle f, g \rangle_\mathfrak{h} \mathbb{1}_\mathcal{F} \tag{2.3}$$

for any $f, g \in \mathfrak{h}$ where $\{A, B\} := AB + BA$ is the anticommutator.

The map $f \mapsto c^*(f)$ is linear and $f \mapsto c(f)$ is antilinear. Furthermore, they are adjoints of each other: $c^*(f) = (c(f))^*$. For any $N \in \mathbb{N}$ and $f_1, \ldots, f_N \in \mathfrak{h}$ the creation operators satisfy

$$c^*(f_1) \cdots c^*(f_N)\Omega = f_1 \wedge \cdots \wedge f_N.$$

The creation and annihilation operators introduced here are a specific representation of the (abstract) CAR (2.3), namely the Fock representation.

Definition 2.19. The C^*-algebra $\mathcal{A}^-$ generated by $\{1, c^*(f), c(f) \big| f \in \mathfrak{h}\}$ is called *CAR algebra*.

Note that the CAR algebra defined here is isomorphic to the Grassmann algebra introduced in Chapter 5, Section 3.

For a given arbitrary ONB $\{\varphi_k\}_{k=1}^{\infty}$ of $\mathfrak{h}$ we here and henceforth use the abbreviations $c_k^* \equiv c^*(\varphi_k)$ and $c_k \equiv c(\varphi_k)$. Using this ONB the set

$$\left\{ c_{k_1}^* \cdots c_{k_N}^* \Omega \,\middle|\, 1 \le k_1 < \cdots < k_N \right\}$$

is an ONB of the N-particle Hilbert space $\mathfrak{h}^{\wedge N}$ and the set

$$\left\{ c_{k_1}^* \cdots c_{k_N}^* \Omega \,\middle|\, N \in \mathbb{N}_0,\ 1 \le k_1 < \cdots < k_N \right\}$$

is an ONB of the fermion Fock space $\mathcal{F}^-$.

For fermions a second quantized operator can be expressed in terms of fermion creation and annihilation operators analogously to the boson case. For a one-particle operator h on $\mathfrak{h}$ and any ONB $\{\varphi_k\}_{k=1}^{\infty}$ of $\mathcal{D}(h)$ the second quantization $\mathbb{h}\big|_{\mathcal{F}^-} := A\mathbb{h}A : \mathcal{D}(\mathbb{h}) \cap \mathcal{F}^- \to \mathcal{F}^-$ restricted to the fermion Fock space can be rewritten as

$$\mathbb{h}\big|_{\mathcal{F}^-} = \sum_{k,l=1}^{\infty} h_{kl}\, c_k^* c_l$$

with $h_{kl} := \langle \varphi_k, h\varphi_l \rangle_{\mathfrak{h}} \in \mathbb{C}$ for all $k, l \in \mathbb{N}$. The second quantization $\mathbb{V}\big|_{\mathcal{F}^-} := A\mathbb{V}A : \mathcal{F}^- \to \mathcal{F}^-$ of a two-particle operator $V : \mathcal{D}(V) \to \mathfrak{h} \otimes \mathfrak{h}$, $\mathcal{D}(V) \subseteq \mathfrak{h} \otimes \mathfrak{h}$ is

$$\mathbb{V}\big|_{\mathcal{F}^-} = \sum_{k,l,m,n=1}^{\infty} V_{kl;mn}\, c_l^* c_k^* c_m c_n$$

where $V_{kl,mn} := \langle \varphi_k \otimes \varphi_l, V(\varphi_m \otimes \varphi_n) \rangle_{\mathfrak{h}\otimes\mathfrak{h}}$ for any $k, l, m, n \in \mathbb{N}$. Here we have to assume that $\varphi_k \otimes \varphi_l \in \mathcal{D}(V)$ for any two elements φ_k, φ_l of the ONB. Therefore, the particle number operator reads

$$\widehat{\mathbb{N}} = \sum_{k=1}^{\infty} c_k^* c_k$$

as a quadratic form for any ONB $\{\varphi_k\}_{k=1}^{\infty}$ of $\mathfrak{h}$.

2.1 States and Density Matrices

As for the bosons the states carry all information about the system while the selfadjoint elements of the CAR algebra, the so-called *observables*, represent physical quantities that can be measured.

Definition 2.20. A continuous linear functionals $\omega \in (\mathcal{A}^-)^*$ is called *state* if it is normalized, $\omega(\mathbb{1}_F) = 1$, and positive, i.e., $\omega(A) \geq 0$ for all positive semi-definite operators $A \in \mathcal{A}^-$.

The fermion systems we are dealing with in this work are particle number conserving. Therefore, we only consider *even* states, i.e., states for which

$$\omega(e(f_1)\cdots e(f_n)) = 0$$

for every odd integer n. Here and henceforth in this section on fermions e denotes either a creation operator c^* or an annihilation operator c. Moreover, the particle number expectation value, as well as its variance are assumed to be finite and we restrict ourselves to the following states:

Definition 2.21. The set of all even states with finite particle number variance is

$$\begin{aligned}\mathcal{Z}^- := \big\{ \omega \in \mathcal{L}(\mathcal{A}^-) \,\big|\, \omega(\mathbb{1}_\mathcal{F}) = 1;\ \omega(A) \geq 0\ \forall\ A \in \mathcal{A}^-,\ A \geq 0; \\ \omega(\widehat{\mathbb{N}}^2) < \infty;\ \omega(e(f_1)\cdots e(f_n)) = 0\ \forall \text{ odd } n \in \mathbb{N} \big\}.\end{aligned}$$

For any $N \in \mathbb{N}$ $\mathcal{Z}_N^- := \left\{ \omega \in \mathcal{Z}^- \,\middle|\, \omega(\widehat{\mathbb{N}}) = N \right\}$ denotes the set of even N-particle states.

In order to ensure that the particle number expectation value is finite, it suffices to require a finite particle number variance since

$$\omega(\widehat{\mathbb{N}}) \leq \sqrt{\omega(\widehat{\mathbb{N}}^2)} < \infty$$

by the Cauchy–Schwarz inequality.

Definition 2.22. The state $\omega \in \mathcal{Z}^-$ is called *pure* if there is a $\Phi \in \mathcal{F}^-$ such that

$$\omega(A) = \langle \Phi, A\Phi \rangle_\mathcal{F}$$

for any $A \in \mathcal{A}^-$.

Definition 2.23. We say that the state $\omega \in \mathcal{Z}^-$ is *quasifree* and write $\omega \in \mathcal{Z}_{\mathrm{qf}}^-$ if ω fulfills Wick's Theorem, i.e.,

$$\begin{aligned}&\omega(e_1 e_2 \cdots e_{2N-1}) = 0 \quad \text{and} \\ &\omega(e_1 e_2 \cdots e_{2N}) = \sum_\pi \omega(e_{\pi(1)} e_{\pi(2)}) \cdots \omega(e_{\pi(2N-1)} e_{\pi(2N)})\end{aligned}$$

for every $N \in \mathbb{N}$ where the sum is over all permutations $\pi \in \mathfrak{S}_{2N}$ satisfying

$$\pi(1) < \pi(3) < \cdots < \pi(2N-1) \text{ and } \pi(2k-1) < \pi(2k)$$

for every $k \in \{1, 2, \dots, N\}$. $\mathcal{Z}^-_{\mathrm{pqf}}$ denotes the subset of all pure quasifree states.

Every *Slater determinant*, i.e., a wave function of the form $f_1 \wedge \cdots \wedge f_N \in \mathcal{F}^-$ with orthonormal $f_1, \dots, f_N \in \mathfrak{h}$ and $N \in \mathbb{N}$, defines a pure quasifree state.

In particular, even states are centered (in a sense analogous to Definition 2.8 for bosons). For bosons the set of centered quasifree states (Remark 2.10) is a proper subset of the set of quasifree states (Definition 2.9), $\mathcal{Z}^+_{\mathrm{cqf}} \subsetneq \mathcal{Z}^+_{\mathrm{qf}}$. For fermions all quasifree states are centered.

Definition 2.24. Let $\rho \in \mathcal{L}^1_+(\mathcal{F})$ have unit trace, i.e., $\mathrm{tr}_{\mathcal{F}}\{\rho\} = 1$. Such trace class operators are called *density matrices*.

For any density matrix $\rho \in \mathcal{L}^1_+(\mathcal{F})$ the map $\mathcal{A}^- \to \mathbb{C}, A \mapsto \langle A \rangle_\rho := \mathrm{tr}_{\mathcal{F}}(\rho A)$ defines a state. The assumption of particle number-conservation can be transferred to density matrices by requiring

$$\rho = \bigoplus_{N=0}^{\infty} \rho^{(N)} \quad \text{and} \quad \langle \widehat{\mathbb{N}}^2 \rangle_\rho < \infty \tag{2.4}$$

with $\rho^{(N)} : \mathfrak{h}^{\wedge N} \to \mathfrak{h}^{\wedge N}$. Note that for any $f_1, \dots, f_m, g_1, \dots, g_n \in \mathfrak{h}$ with $m, n \in \mathbb{N}, m \neq n$,

$$\mathrm{tr}_{\mathcal{F}}(\rho\, c^*(f_1) \cdots c^*(f_m) c(g_1) \cdots c(g_n)) = 0.$$

For every state $\omega \in \mathcal{Z}^-$ there is a density matrix $\rho \in \mathcal{L}^1_+(\mathcal{F})$ fulfilling (2.4) and $\mathrm{tr}(\rho A) = \omega(A)$ for all $A \in \mathcal{A}^-$.

2.2 One- and Two-Particle Density Matrices and Representability

Definition 2.25. For any state $\omega \in \mathcal{Z}^-$ we define the *(fermion) one-particle density matrix* (1-pdm) $\gamma_\rho \in \mathcal{B}(\mathfrak{h})$ and the *two-particle density matrix* (2-pdm) $\Gamma_\omega \in \mathcal{B}(\mathfrak{h} \otimes \mathfrak{h})$ by

$$\langle f_1, \gamma_\omega g_1 \rangle_{\mathfrak{h}} := \omega(c^*(g_1) c(f_1)) \text{ and}$$
$$\langle f_1 \otimes f_2, \Gamma_\omega (g_1 \otimes g_2) \rangle_{\mathfrak{h} \otimes \mathfrak{h}} := \omega(c^*(g_2) c^*(g_1) c(f_1) c(f_2))$$

for any $f_1, f_2, g_1, g_2 \in \mathfrak{h}$.

With the exchange operator $\mathrm{Ex} \in \mathcal{B}(\mathfrak{h} \otimes \mathfrak{h})$ given by

$$\mathrm{Ex}\,(f \otimes g) := g \otimes f$$

for any $f, g \in \mathfrak{h}$ the CAR yields the antisymmetry property of Γ_ω:

$$\mathrm{Ex}\Gamma_\omega = -\Gamma_\omega = \Gamma_\omega \mathrm{Ex}.$$

For any state $\omega \in \mathcal{Z}^-$ the 1-pdm satisfies

$$\gamma_\omega \in \mathcal{L}^1(\mathfrak{h}) \,, \quad 0 \le \gamma_\omega \le \mathbb{1}_{\mathfrak{h}} \,, \quad \text{and} \quad \mathrm{tr}_{\mathfrak{h}}\left(\gamma_\omega\right) = \omega(\widehat{\mathbb{N}})$$

and the 2-pdm

$$\begin{aligned} &\Gamma_\omega \in \mathcal{L}^1(\mathfrak{h} \otimes \mathfrak{h}) \,, \quad 0 \le \Gamma_\omega \le \omega(\widehat{\mathbb{N}}) \mathbb{1}_{\mathfrak{h}\otimes\mathfrak{h}} \,, \\ &\text{and } \mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\Gamma_\omega\right) = \omega\big(\widehat{\mathbb{N}}\big(\widehat{\mathbb{N}} - \mathbb{1}_{\mathcal{F}}\big)\big). \end{aligned}$$

Assuming $\omega \in \mathcal{Z}_N^-$ we have

$$\langle f, \gamma_\gamma g \rangle_{\mathfrak{h}} = \frac{1}{N-1} \sum_{k=1}^{\infty} \langle f \otimes \varphi_k, \Gamma_\omega \left(g \otimes \varphi_k\right) \rangle_{\mathfrak{h}\otimes\mathfrak{h}}$$

for all $f, g \in \mathfrak{h}$ where $\{\varphi_k\}_{k=1}^{\infty}$ denotes an ONB of $\mathfrak{h}$.
If and only if $\omega \in \mathcal{Z}^-$ is a pure state with $\omega(\cdot) = \langle \Psi, (\cdot)\, \Psi \rangle_{\mathcal{F}}$ where $\Psi := c^*(f_1) \cdots c^*(f_N)\Omega$ with $f_1, \ldots, f_N \in \mathfrak{h}$ is a Slater determinant, the 1-pdm fulfills

$$\gamma_\omega = \sum_{i=1}^{N} |f_i\rangle \langle f_i| \,.$$

In this case the 2-pdm is completely determined by the 1-pdm:

$$\Gamma_\omega = \left(\mathbb{1}_{\mathfrak{h}\otimes\mathfrak{h}} - \mathrm{Ex}\right) \left(\gamma_\omega \otimes \gamma_\omega\right).$$

Definition 2.26. A pair (γ, Γ) of operators on $\mathfrak{h} \times (\mathfrak{h} \otimes \mathfrak{h})$ is called *representable* if there is a state $\omega \in \mathcal{Z}^-$ with $\gamma_\omega = \gamma$ and $\Gamma_\omega = \Gamma$. If we restrict our attention to N-particle states, i.e.,$\mathcal{Z}_N^-$, with a given $N \in \mathbb{N}$, we call the a representable pair *N-representable*. Necessary conditions on the pair $(\gamma, \Gamma)$to be representable, are called *representability conditions*.

The properties given in the following definition are the basic representability conditions.

Definition 2.27. The pair (γ, Γ) of operators on $\mathfrak{h} \times (\mathfrak{h} \otimes \mathfrak{h})$ is called *admissible* if

(i) Γ is antisymmetric, i.e., $\mathrm{Ex}\Gamma = \Gamma\,\mathrm{Ex} = -\Gamma$, selfadjoint, and $\Gamma \in \mathcal{L}^1\left(\mathfrak{h} \otimes \mathfrak{h}\right)$, and

(ii) γ is selfadjoint, positive semi-definite and bounded by 1, i.e., $0 \le \gamma \le \mathbb{1}_{\mathfrak{h}}$, and $\gamma \in \mathcal{L}^1\left(\mathfrak{h}\right)$ with $\mathrm{tr}_{\mathfrak{h}}\left(\gamma\right) = \omega\left(\widehat{\mathbb{N}}\right)$.

2.3 Generalized One-Particle Density Matrices

In [BLS94] a generalization of the one-particle density matrix was introduced. We recall this definition and state some basic properties, but refer the reader to [BLS94] and [Sol07] for a more detailed survey. As for bosons we use a notation in which the defined objects depend on the specific choice of the ONB of $\mathfrak{h}$. The complex conjugates of a function and an operator are defined as in Subsection 1.4. A basis-independent formulation can be found in [Sol07].

Definition 2.28. Let $\{\varphi_k\}_{k=1}^{\infty}$ be an ONB of $\mathfrak{h}$. The *generalized one-particle density matrix* $\widetilde{\gamma}_\omega : \mathfrak{h} \oplus \mathfrak{h} \to \mathfrak{h} \oplus \mathfrak{h}$ of a state $\omega \in \mathcal{Z}^-$ is defined by

$$\langle (f_1 \oplus f_2), \widetilde{\gamma}_\omega (g_1 \oplus g_2) \rangle := \omega\big([c^*(g_1) + c(\overline{g}_2)] \, [c(f_1) + c^*(\overline{f}_2)] \big)$$

for $f_1, f_2, g_1, g_2 \in \mathfrak{h}$.

With the operator $\alpha_\omega^* : \mathfrak{h} \to \mathfrak{h}$ given for every $f, g \in \mathfrak{h}$ by

$$\langle f, \alpha_\omega^* g \rangle := \omega\big(c^*(g)\, c^*(\overline{f})\big)$$

the generalized 1-pdm can be expressed as

$$\widetilde{\gamma}_\omega = \begin{pmatrix} \gamma_\omega & \alpha_\omega \\ \alpha_\omega^* & \mathbb{1}_{\mathfrak{h}} - \overline{\gamma}_\omega \end{pmatrix}.$$

Note that α is antisymmetric, i.e., $\alpha^T = -\alpha$, as follows from CAR.

A further generalization of the 1-pdm and a generalization of the 2-pdm like the ones for bosons (see Chapter 3, Definitions 3.25 and 3.29) do not yield new information for the system: Since the fermion states are assumed to be even, the matrices obtained by such generalizations have a block-diagonal structure. The independent conditions on the 1- and 2-pdm obtained from these matrices are exactly the admissibility and the G-, P-, and Q-condition specified in Chapter 4, Section 3.

3 Bogoliubov Transformations

The Bogoliubov transformations are the equivalent of a change of coordinates known from Linear Algebra. Therefore, we require that the transformed creation and annihilation operators fulfill the CCR for bosons and the CAR for fermions.

This section follows the lecture notes of Solovej [Sol07] in defining the Bogoliubov transformations. For reasons of consistency, we customize the notation to the one used throughout this work. We choose an ONB $\{\varphi_k\}_{k=1}^{\infty}$ of $\mathfrak{h}$. As before, the complex conjugate of a function f is given as $\overline{f} := \sum_{k=1}^{\infty} \overline{\mu}_k \varphi_k$ if $f = \sum_{k=1}^{\infty} \mu_k \varphi_k$. Moreover, the complex conjugate $\overline{A}$ of an operator A is defined by $\langle f, \overline{A} g \rangle_{\mathfrak{h}} := \overline{\langle \overline{f}, A \overline{g} \rangle_{\mathfrak{h}}}$ and the transpose of A is $A^T := \overline{A^*}$. Therefore, the objects defined subsequently depend on the choice of the ONB. A basis-independent formulation is given in [Sol07].

3.1 Boson Bogoliubov Transformations

Definition 2.29. A linear map $U = \left(\begin{smallmatrix} u & v \\ \overline{v} & \overline{u} \end{smallmatrix}\right) : \mathfrak{h} \oplus \mathfrak{h} \to \mathfrak{h} \oplus \mathfrak{h}$ is called *(boson) Bogoliubov transformation* if the two linear operators $u : \mathfrak{h} \to \mathfrak{h}$ and $v : \mathfrak{h} \to \mathfrak{h}$ fulfill

$$
\begin{aligned}
uu^* - vv^* &= \mathbb{1}_{\mathfrak{h}}, \\
u^*u - v^T\overline{v} &= \mathbb{1}_{\mathfrak{h}}, \\
u^*v - v^T\overline{u} &= 0, \\
uv^T - vu^T &= 0.
\end{aligned}
$$

The conditions on u and v from the definition are equivalent to the two conditions

$$U^*\mathcal{S}U = \mathcal{S} \qquad \text{and} \qquad U\mathcal{S}U^* = \mathcal{S}.$$

A further equivalent statement is

$$\langle UF_1, \mathcal{S}UF_2\rangle_{\mathfrak{h}\oplus\mathfrak{h}} = \langle F_1, \mathcal{S}F_2\rangle_{\mathfrak{h}\oplus\mathfrak{h}}$$

for every $F_1, F_2 \in \mathfrak{h} \oplus \mathfrak{h}$. Therefore, the inverse of a Bogoliubov transformation is

$$U^{-1} = \mathcal{S}U^*\mathcal{S},$$

where

$$\mathcal{S} := \begin{pmatrix} \mathbb{1}_{\mathfrak{h}} & 0 \\ 0 & -\mathbb{1}_{\mathfrak{h}} \end{pmatrix},$$

and itself a boson Bogoliubov transformation.

Lemma 2.30. *For a boson Bogoliubov transformation $U = \left(\begin{smallmatrix} u & v \\ \overline{v} & \overline{u} \end{smallmatrix}\right) : \mathfrak{h} \oplus \mathfrak{h} \to \mathfrak{h} \oplus \mathfrak{h}$ there is a unitary transformation $\mathbb{U}_U : \mathcal{F}^+ \to \mathcal{F}^+$ fulfilling*

$$\mathbb{U}_U \left[a^*(f) + a(\overline{g})\right] \mathbb{U}_U^* = a^*(uf + v\overline{g}) + a(\overline{v}\overline{f} + \overline{u}g)$$

for all $f, g \in \mathfrak{h}$ if and only if U fulfills the Shale–Stinespring condition, i.e., if v^*v is trace class. The map $\mathbb{U}_U$ is called unitary representation or implementation on the Fock space.

The conditions on u and v from Definition 2.29 ensure that the transformed creation and annihilation operators, which are given by $b^*(f) := \mathbb{U}_U a^*(f)\mathbb{U}_U^*$ and consequently $b(f) = \mathbb{U}_U a(f)\mathbb{U}_U^*$ for every $f \in \mathfrak{h}$, satisfy the CCR.

3.1.1 Bogoliubov–Weyl transformation

We extend the Bogoliubov transformation slightly. Therefore, we merge the unitary Weyl transformation (see Subsection 1.1) and the boson Bogoliubov transformation. This more general map is obtained by a translation of the creation or annihilation operator with a Weyl operator and afterwards mixing the creation and annihilation operators by a Bogoliubov transformation.

Definition 2.31. Let $\phi \in \mathfrak{h}$ and $U = \left(\begin{smallmatrix} u & v \\ \overline{v} & \overline{u} \end{smallmatrix}\right) : \mathfrak{h} \oplus \mathfrak{h} \to \mathfrak{h} \oplus \mathfrak{h}$ with $v \in \mathcal{L}^2(\mathfrak{h})$ be a Bogoliubov transformation. The *Bogoliubov–Weyl transformation* is defined by

$$\mathbb{U}_{\phi,U} a(f) \mathbb{U}_{\phi,U}^* := a(uf) + a^*(v\overline{f}) + \langle f, \phi \rangle \, \mathbb{1}_{\mathcal{F}}$$

for any $f \in \mathfrak{h}$. The map $\mathbb{U}_{\phi,U} : \mathcal{F}^+ \to \mathcal{F}^+$ is unitary and $\mathbb{U}_{\phi,U} = \mathbb{U}_U \mathbb{W}_\phi$.

We consequently have $\mathbb{U}_{\phi,U} a^*(f) \mathbb{U}_{\phi,U}^* = a^*(uf) + a(v\overline{f}) + \langle \phi, f \rangle \, \mathbb{1}_{\mathcal{F}}$.

3.2 Fermion Bogoliubov Transformations

Analogously we have for fermions:

Definition 2.32. Let $u : \mathfrak{h} \to \mathfrak{h}$ and $v : \mathfrak{h} \to \mathfrak{h}$ be two linear maps that satisfy

$$\begin{aligned} uu^* + vv^* &= \mathbb{1}, \\ u^* u + v^T \overline{v} &= \mathbb{1}, \\ u^* v + v^T \overline{u} &= 0, \\ uv^T + vu^T &= 0. \end{aligned}$$

Then the linear map $U := \left(\begin{smallmatrix} u & v \\ \overline{v} & \overline{u} \end{smallmatrix}\right) : \mathfrak{h} \oplus \mathfrak{h} \to \mathfrak{h} \oplus \mathfrak{h}$ is called *fermion Bogoliubov transformation*.

The conditions on u and v are necessary and sufficient conditions that U is unitary, i.e.,

$$U^* U = \mathbb{1}_{\mathfrak{h} \oplus \mathfrak{h}} \qquad \text{and} \qquad UU^* = \mathbb{1}_{\mathfrak{h} \oplus \mathfrak{h}},$$

what is also equivalent to

$$\langle UF_1, UF_2 \rangle_{\mathfrak{h} \oplus \mathfrak{h}} = \langle F_1, F_2 \rangle_{\mathfrak{h} \oplus \mathfrak{h}}$$

for every $F_1, F_2 \in \mathfrak{h} \oplus \mathfrak{h}$. Thus, the inverse of a fermion Bogoliubov transformation U is the fermion Bogoliubov transformation U^*.

Lemma 2.33. *Let $U = \left(\begin{smallmatrix} u & v \\ \overline{v} & \overline{u} \end{smallmatrix}\right) : \mathfrak{h} \oplus \mathfrak{h} \to \mathfrak{h} \oplus \mathfrak{h}$ be a fermion Bogoliubov transformation. There is a unitary transformation $\mathbb{U}_U : \mathcal{F}^- \to \mathcal{F}^-$ with*

$$\mathbb{U}_U \left[c^*(f) + c(\overline{g}) \right] \mathbb{U}_U^* = c^*(uf + vg) + c(\overline{v}\overline{f} + \overline{u}\overline{g})$$

for all $f \oplus g \in \mathfrak{h} \oplus \mathfrak{h}$ if and only if $v^* v$ is trace class. This condition on v is called Shale-Stinespring condition.

The transformed creation and annihilation operators, which are given by $b^*(f) := \mathbb{U}_U c^*(f) \mathbb{U}_U^*$ and, thus, $b(f) = \mathbb{U}_U c(f) \mathbb{U}_U^*$ for any $f \in \mathfrak{h}$, satisfy the CAR due to the conditions imposed on u and v in Definition 2.32. Since we assume fermion systems to be particle number-conserving, we do not need a Weyl transformation and consequently Bogoliubov–Weyl transformation for fermions.

4 Bogoliubov–Hartree–Fock Theory

The Bogoliubov–Hartree–Fock theory, for fermions also called generalized Hartree–Fock theory and for bosons Bogoliubov variational theory, is a method to approximate ground state energies, as well as ground states of a given Hamiltonian $\mathbb{H}$ on $\mathcal{F}^{\pm}$. In this work we focus on an approximation of the ground state energy $E_{\mathrm{gs}} := \inf\{\sigma(\mathbb{H})\}$.

For a more detailed discussion of the Bogoliubov–Hartree–Fock theory for fermions we refer the reader to [BLS94] and for bosons to [Sol06, Nam11].

4.1 Boson Bogoliubov–Hartree–Fock Theory

Since most boson systems do not conserve the particle number, an approximation method is required where the particle number is not fixed in the variational process. The Rayleigh–Ritz principle allows us to determine the ground state energy by the variation

$$E_{\mathrm{gs}} = \inf\left\{\omega(\mathbb{H})\middle|\,\omega \in \mathcal{Z}^{+}\right\}.$$

Since an exact calculation of this energy is only possible for very few systems, we have to restrict the variation obtaining an upper bound for the ground state energy. The Bogoliubov–Hartree–Fock (BHF) theory is based on such a restriction of the variation, namely the restriction to quasifree states. So the Bogoliubov–Hartree–Fock energy is

$$E_{\mathrm{BHF}} := \inf\left\{\omega(\mathbb{H})\middle|\,\omega \in \mathcal{Z}^{+}_{\mathrm{qf}}\right\}.$$

Recall that a quasifree boson state $\omega \in \mathcal{Z}^{+}_{\mathrm{qf}}$ is not necessarily centered and note that any quasifree state is uniquely determined by its first moment b_ω and its generalized 1-pdm $\widetilde{\gamma}_\omega$, see [Sol06, Nam11, BBKM13]. Thus, we can define an energy functional $\mathcal{E}_{\mathrm{BHF}} : \mathcal{D}(\mathcal{E}_{\mathrm{BHF}}) \to \mathbb{C}$, $\mathcal{D}(\mathcal{E}_{\mathrm{BHF}}) \subseteq \mathcal{B}(\mathfrak{h} \oplus \mathfrak{h}) \times \mathfrak{h}$ by $\mathcal{E}_{\mathrm{BHF}}(\widetilde{\gamma}_\omega, b_\omega) := \omega(\mathbb{H})$. Then we have

$$\begin{aligned} E_{\mathrm{BHF}} &= \inf\left\{\mathcal{E}_{\mathrm{BHF}}(\widetilde{\gamma}_\omega, b_\omega)\middle|\,\omega \in \mathcal{Z}^{+}_{\mathrm{qf}}\right\} \\ &= \inf\left\{\mathcal{E}_{\mathrm{BHF}}(\widetilde{\gamma}, b)\middle|\, b \in \mathfrak{h};\ \widetilde{\gamma} \in \mathcal{B}(\mathfrak{h} \oplus \mathfrak{h}) \text{ with } \widetilde{\gamma} \geq 0,\ \mathrm{tr}(\gamma) < \infty\right\}. \end{aligned}$$

Here, we used that any quasifree state is uniquely linked to a centered quasifree state with the Weyl transformation $\mathbb{W}_b$ for a $b \in \mathfrak{h}$, namely its first moment, and that any positive semi-definite operator $\widetilde{\gamma} \equiv \begin{pmatrix} \gamma & \alpha \\ \alpha^* & \mathbb{1}_{\mathfrak{h}} + \overline{\gamma} \end{pmatrix}$: $\mathfrak{h} \oplus \mathfrak{h} \to \mathfrak{h} \oplus \mathfrak{h}$ with $\mathrm{tr}(\gamma) \leq \infty$ is the generalized 1-pdm of a unique centered quasifree state, cf. [Sol06, Nam11, BBKM13].

4.2 Fermion Bogoliubov–Hartree–Fock Theory

The standard examples for fermion systems which should be covered in this work are atoms and molecules in the Born–Oppenheimer approximation. The Hamiltonian of such a system with N electrons is the selfadjoint operator on $\mathfrak{h}^{\wedge N}$ given by

$$H^{(N)} := \sum_{i=1}^{N} [-\Delta_i - U(x_i)] + \sum_{1 \le i < j \le N} V(x_i, x_j)$$

where Δ_i is the Laplace operator acting on the space of the i-th electron and $x_i \in \mathbb{R}^3$, $1 \le i \le N$. U is an external potential, usually the attraction between electrons and nuclei, which are on fixed positions in the Born–Oppenheimer approximation, and V the repulsive interaction between two electrons. The multiplication operators associated to these potentials we also denote by U and V, respectively. This Hamiltonian can be extended to the fermion Fock space and then reads

$$\mathbb{H} := \sum_{i,j=1}^{\infty} h_{ij} c_i^* c_j + \frac{1}{2} \sum_{i,j,k,l=1}^{\infty} V_{ij,kl} c_j^* c_i^* c_k c_l.$$

The one-particle operator h and the pair-interaction operator V are defined by

$$h_{ij} := \langle \varphi_i, (-\Delta - U)\, \varphi_j \rangle_{\mathfrak{h}} \text{ and}$$
$$V_{ij,kl} := \langle \varphi_i \otimes \varphi_j, V\, (\varphi_k \otimes \varphi_l) \rangle_{\mathfrak{h} \otimes \mathfrak{h}},$$

respectively, for any elements of a given ONB $\{\varphi_i\}_{i=1}^{\infty}$ of $\mathfrak{h}$ with $\|\nabla \varphi_i\|_{\mathfrak{h}} < \infty$. The ground state energy of this Hamiltonian can be determined using the Rayleigh–Ritz principle:

$$E_{\text{gs}} = \inf \left\{ \omega(\mathbb{H}) \,\middle|\, \omega \in \mathcal{Z}^- \right\}.$$

Defining

$$\mathcal{E}(\gamma, \Gamma) := \text{tr}(h\gamma) + \frac{1}{2} \text{tr}(V\Gamma),$$

we obtain

$$E_{\text{gs}} = \inf \left\{ \mathcal{E}(\gamma, \Gamma) \,\middle|\, (\gamma, \Gamma) \text{ is representable} \right\}$$

where the problem of representability arises: *Is there a (simple) classification of all representable operator pairs* (γ, Γ) *on* $\mathfrak{h} \times (\mathfrak{h} \otimes \mathfrak{h})$*?*

Up to today this question waits for its answer. Thus, an important topic in quantum chemistry is the approximation of the ground state energy of an atom or molecule. The Bogoliubov–Hartree–Fock energy

$$E_{\text{BHF}} := \inf \left\{ \omega(\mathbb{H}) \,\middle|\, \omega \in \mathcal{Z}_{\text{qf}}^- \right\}$$

yields an upper bound to the ground state energy E_{gs}. Since we assume the fermion system to be particle number-conserving, we know that the quasifree fermion states are, in particular, centered and are uniquely determined by their generalized 1-pdm.

In defining the Bogoliubov–Hartree–Fock functional $\mathcal{E}_{\mathrm{BHF}}$ by

$$\mathcal{E}_{\mathrm{BHF}}(\widetilde{\gamma}_{\omega}) := \omega(\mathbb{H})$$

for any quasifree state ω with generalized 1-pdm $\widetilde{\gamma}_{\omega}$ we can write

$$E_{\mathrm{BHF}} = \inf \left\{ \mathcal{E}_{\mathrm{BHF}}(\widetilde{\gamma}) \middle| \widetilde{\gamma} \geq 0,\ \mathrm{tr}_{\mathfrak{h}}(\gamma) < \infty \right\}.$$

This is the starting point of our further survey in Subsection 4.2 of Chapter 3.

Chapter 3

Generalized One-Particle Density Matrices and Quasifree States

This chapter is a joint work with Volker Bach, Sébastien Breteaux, and Edmund Menge and a revised version of the article [BBKM13].

1 Introduction

The Rayleigh–Ritz variational principle for the ground state energy is the starting point of many computations and approximations in quantum chemistry. For a many-particle system, whose dynamics is generated by a Hamiltonian $\mathbb{H}$, it can be written as

$$E_{gs} = \inf \left\{ \mathrm{tr}_{\mathcal{F}}(\rho \mathbb{H}) \middle| \rho \geq 0,\ \mathrm{tr}_{\mathcal{F}}(\rho) = 1 \right\} \tag{3.1}$$

where ρ varies over the density matrices on the Fock space $\mathcal{F}^{\pm} \equiv \mathcal{F}^{\pm}[\mathfrak{h}]$ of the system (E_{gs} in (3.1) is actually the *total* ground state energy in the grand canonical ensemble). A typical many-particle Hamiltonian is given as the sum $\mathbb{H} = \mathbb{h} + \mathbb{V}$ of the second quantization $\mathbb{h}$ of a one-particle operator h and the second quantization $\mathbb{V}$ of a pair potential V. Since $\mathbb{h}$ is quadratic and $\mathbb{V}$ is quartic in the field operators, one can rewrite (3.1) in terms of the one-particle density matrix $\gamma_\rho \in \mathcal{L}^1_+(\mathfrak{h})$ and the two-particle density matrix $\Gamma_\rho \in \mathcal{L}^1_+(\mathfrak{h} \otimes \mathfrak{h})$ of a given density matrix $\rho \in \mathcal{L}^1_+(\mathcal{F})$ as

$$E_{gs} = \inf \left\{ \mathcal{E}(\gamma_\rho, \Gamma_\rho) \middle| \rho \geq 0,\ \mathrm{tr}_{\mathcal{F}}(\rho) = 1 \right\}$$

where the energy functional $\mathcal{E}$ is defined by

$$\mathcal{E}(\gamma_\rho, \Gamma_\rho) := \mathrm{tr}_{\mathfrak{h}}(h\gamma_\rho) + \frac{1}{2}\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}(V\Gamma_\rho).$$

The computation of the ground state energy and the corresponding ground state vector of a quantum mechanical many-particle system is a complex, if not impossible, task and one resorts to approximation methods. The Hartree–Fock approximation is one of the first approximations that emerged from ground state computations in quantum chemistry, cf. [Bac92, BLS94, BKM12].

In its original formulation the Rayleigh–Ritz principle for the ground state energy in terms of wave functions,

$$E_{\mathrm{gs}} = \inf\Big\{ \langle \Psi, \mathbb{H}\Psi\rangle_{\mathcal{F}} \,\Big|\, \Psi \in \mathcal{F},\ \|\Psi\|_{\mathcal{F}} = 1\Big\},$$

of a fermion system with Hamiltonian $\mathbb{H}$ is replaced by a variation over Slater determinants,

$$E_{\mathrm{hf}} = \inf\Big\{ \langle \Phi, \mathbb{H}\Phi\rangle_{\mathcal{F}} \,\Big|\, N \in \mathbb{N},\ \Phi = \varphi_1 \wedge \cdots \wedge \varphi_N,\ \langle \varphi_i, \varphi_j\rangle_{\mathfrak{h}} = \delta_{i,j}\Big\} \quad (3.2)$$

where the Hamiltonian $\mathbb{H}$ conserves the particle number, i.e., $[\mathbb{H}, \widehat{\mathbb{N}}] = 0$ with $\widehat{\mathbb{N}}$ being the particle number operator. The density matrix $\rho = |\Phi\rangle\langle\Phi|$ associated to a Slater determinant is a pure, particle number-conserving, quasifree state and (3.2) can be rewritten as

$$E_{\mathrm{hf}} = \inf\Big\{ \mathrm{tr}_{\mathcal{F}}(\rho\mathbb{H} \,\Big|\, \rho \text{ is a pure, particle number-conserving, quasifree density matrix}\Big\}.$$

Since the one-particle density matrix γ of a fermion Slater determinant, $\Phi = \varphi_1 \wedge \cdots \wedge \varphi_N$ with $N \in \mathbb{N}$, is the rank-N orthogonal projection onto $\mathrm{span}\{\varphi_1, \ldots, \varphi_N\}$ and its two-particle density matrix is given as $\Gamma = (\mathbb{1}_{\mathfrak{h}\otimes\mathfrak{h}} - \mathrm{Ex})(\gamma \otimes \gamma)$, the Hartree–Fock energy can be written as

$$E_{\mathrm{hf}} = \inf\Big\{ \mathcal{E}\big(\gamma, (\mathbb{1}_{\mathfrak{h}\otimes\mathfrak{h}} - \mathrm{Ex})(\gamma\otimes\gamma)\big) \,\Big|\, \gamma = \gamma^2 = \gamma^*,\ \mathrm{tr}_{\mathfrak{h}}(\gamma) < \infty\Big\}.$$

In case of purely repulsive pair potentials V Lieb's variational principle [Lie81, Bac92, BLS94] asserts that

$$E_{\mathrm{hf}} = \inf\Big\{ \mathcal{E}\big(\gamma, (\mathbb{1}_{\mathfrak{h}\otimes\mathfrak{h}} - \mathrm{Ex})(\gamma\otimes\gamma)\big) \,\Big|\, 0 \le \gamma \le \mathbb{1}_{\mathfrak{h}},\ \mathrm{tr}_{\mathfrak{h}}(\gamma) = N\Big\}.$$

Going back to a description on the Fock space, Lieb's variational principle reads

$$E_{\mathrm{hf}} = \inf\Big\{ \mathrm{tr}_{\mathcal{F}}(\rho\mathbb{H}) \,\Big|\, \rho \text{ is a particle number-conserving quasifree density matrix}\Big\}, \quad (3.3)$$

i.e., it asserts that the pureness requirement of the quasifree density matrix can be dropped. As was shown in [BLS94], the property $[\rho, \widehat{\mathbb{N}}] = 0$ of particle number conservation is also obsolete for repulsive pair potentials V and the Hartree–Fock energy E_{hf} agrees with the Bogoliubov–Hartree–Fock energy E_{BHF} defined by

$$E_{\mathrm{BHF}} := \inf\Big\{ \mathrm{tr}_{\mathcal{F}}(\rho\mathbb{H}) \,\Big|\, \rho \text{ is a quasifree density matrix}\Big\}. \quad (3.4)$$

Our first main result is a generalization of Lieb's variational principle (3.3) in several ways. Namely, we show that the infimum in (3.4) is already obtained from a variation over *pure* quasifree density matrices,

$$E_{\mathrm{BHF}} = E_{\mathrm{BHF}}^{\mathrm{pure}} := \inf \Big\{ \mathrm{tr}_{\mathcal{F}}(\rho \mathbb{H}) \Big| \, \rho \text{ is a pure, quasifree density matrix} \Big\},$$

under the mere assumption that $\mathbb{H}$ is bounded below. Neither repulsiveness of the pair potential V nor the form $\mathbb{H} = \mathbb{h} + \mathbb{V}$ or even the conservation of the particle number by $\mathbb{H}$ is assumed. Furthermore, we show that $E_{\mathrm{BHF}} = E_{\mathrm{BHF}}^{\mathrm{pure}}$ for both fermion and boson systems. The precise formulation of this first result and its proof is given in Theorem 3.53. Note that, especially for boson systems, it is crucial that our result does not require the Hamiltonian to conserve the particle number because for most physically interesting models such an assumption would not be fulfilled.

The above result, i.e., Theorem 3.53, brings pure quasifree density matrices ρ into focus. These are fully characterized by their generalized one-particle density matrix $\widetilde{\gamma}_\rho$ defined in terms of their two-point correlation functions as

$$\langle f_1 \oplus f_2, \widetilde{\gamma}_\rho (g_1 \oplus g_2) \rangle_{\mathfrak{h} \oplus \mathfrak{h}} := \mathrm{tr}_{\mathcal{F}} \Big(\rho \, [a^*(g_1) + a(\overline{g}_2)] \, [a(f_1) + a^*(\overline{f}_2)] \Big)$$

where $\{ a^*(f), a(f) \,|\, f \in \mathfrak{h} \}$ are the usual boson or fermion creation operators on $\mathcal{F}^\pm$ fulfilling the canonical commutation or anticommutation relations, respectively, on the symmetric or antisymmetric Fock space $\mathcal{F}^\pm$ with $a(f)$ annihilating the vacuum and $f \mapsto J(f) =: \bar{f}$ being (a fixed antilinear involution on $\mathfrak{h}$ which we refer to as) the complex conjugation. Here we implicitly assume $\mathrm{tr}_{\mathcal{F}}(\rho \, a(f)) = 0$ for all $f \in \mathfrak{h}$, i.e., that ρ is *centered*. This assumption is irrelevant for fermion systems and made without loss of generality for boson systems, as is explained below. The higher correlation of the (centered) quasifree density matrix ρ can be computed from sums over products of the two-point correlation function, i.e., in terms of $\widetilde{\gamma}_\rho$, using Wick's Theorem. It is well-known [BLS94, Sol06] that, as a (2×2)-matrix with operator-valued entries, $\widetilde{\gamma}_\rho$ can be written as

$$\widetilde{\gamma}_\rho = \begin{pmatrix} \gamma_\rho & \alpha_\rho \\ \overline{\alpha}_\rho & \mathbb{1}_{\mathfrak{h}} \pm \overline{\gamma}_\rho \end{pmatrix}, \qquad \gamma_\rho = \gamma_\rho^*, \quad \alpha_\rho = \pm \alpha_\rho^T \tag{3.5}$$

where "+" holds for boson and "−" for fermion systems, and $\overline{A} := JAJ$ denotes the complex conjugate and $A^T := \overline{A}^*$ the transpose of a bounded operator $A \in \mathcal{B}(\mathfrak{h})$. It is easy to check that

$$\widetilde{\gamma}_\rho \geq 0 \qquad \text{for boson systems,} \tag{3.6}$$

$$0 \leq \widetilde{\gamma}_\rho \leq \mathbb{1}_{\mathfrak{h} \oplus \mathfrak{h}} \qquad \text{for fermion systems.} \tag{3.7}$$

We restrict our attention to density matrices with finite particle number expectation for which

$$\mathrm{tr}_{\mathfrak{h}}(\gamma_\rho) = \mathrm{tr}_{\mathcal{F}}(\rho \, \widehat{\mathbb{N}}) < \infty.$$

In this case it is well-known that the converse of (3.6) and (3.7) holds true in the sense that, given $\widetilde{\gamma}$ as in (3.5) with $\gamma = \gamma^* \in \mathcal{L}^1(\mathfrak{h})$, $\gamma \geq 0$, $\alpha = \pm\alpha^T$, and obeying

$$\begin{aligned} \widetilde{\gamma} \geq 0 \qquad & \text{for boson systems,} \\ 0 \leq \widetilde{\gamma} \leq \mathbb{1}_{\mathfrak{h}\oplus\mathfrak{h}} \qquad & \text{for fermion systems,} \end{aligned}$$

there exists a centered quasifree density matrix $\rho \in \mathcal{L}^1_+(\mathcal{F})$ such that

$$\widetilde{\gamma} = \widetilde{\gamma}_\rho.$$

It is furthermore well-known [BLS94, Sol06] that, if ρ is a pure, quasifree density matrix, then

$$\widetilde{\gamma}_\rho = \widetilde{\gamma}_\rho^2 \qquad \text{for fermion systems and} \tag{3.8}$$

$$\widetilde{\gamma}_\rho = -\widetilde{\gamma}_\rho \mathcal{S} \widetilde{\gamma}_\rho \qquad \text{for boson systems} \tag{3.9}$$

where

$$\mathcal{S} = \begin{pmatrix} \mathbb{1}_{\mathfrak{h}} & 0 \\ 0 & -\mathbb{1}_{\mathfrak{h}} \end{pmatrix}.$$

Our second main result is the converse statement: If the generalized one-particle density matrix $\widetilde{\gamma}_\rho$ of a density matrix ρ fulfills (3.8) in the fermion case or (3.9) in the boson case, then the density matrix is a pure, quasifree state. Note that the quasifreeness of ρ is asserted and not assumed. The precise formulation of this result is given in Theorem 3.60.

As our third result we derive representability conditions on the two-particle density matrix Γ_ρ of a boson density matrix ρ. Similar to G-, P-, and Q-conditions for fermion reduced density matrices these conditions follow from the positivity

$$\mathrm{tr}_{\mathcal{F}}\left(\rho P_2^*(a^*, a) P_2(a^*, a)\right) \geq 0 \tag{3.10}$$

of the expectation value of positive semi-definite observables of the form $P_2^*(a^*, a)P_2(a^*, a)$, where $P_2(a^*, a)$ is a polynomial of degree 2 or smaller in the creation and annihilation operators with respect to the density matrix ρ. A crucial difference, however, is that ρ is not assumed to be particle number-conserving as this would not be a fair assumption for boson systems. Hence, the reduction of the general condition (3.10) to simpler conditions like G, P, and Q is not as straightforward as in the fermion case and is in fact not carried out in this paper, but is subject to future work.

2 Second Quantization and the Bogoliubov–Hartree–Fock Theory

Let $\left(\mathfrak{h}, \langle\cdot,\cdot\rangle_{\mathfrak{h}}\right)$ be a complex separable Hilbert space with the inner product $\langle\cdot,\cdot\rangle_{\mathfrak{h}} : \mathfrak{h} \times \mathfrak{h} \to \mathbb{C}$. For any $N \in \mathbb{N}$ the N-particle Hilbert space representing a physical system of N indistinguishable particles is given as the N-fold tensor product of copies of $\mathfrak{h}$, i.e.,

$$\mathfrak{h}^{\otimes N} := \bigotimes^N \mathfrak{h}.$$

The inner product $\langle \cdot, \cdot \rangle_{\mathfrak{h}^{\otimes N}} : \mathfrak{h}^{\otimes N} \times \mathfrak{h}^{\otimes N} \to \mathbb{C}$ is given by

$$\left\langle f^{(N)}, g^{(N)} \right\rangle_{\mathfrak{h}^{\otimes N}} := \prod_{k=1}^{N} \langle f_k, g_k \rangle_{\mathfrak{h}}$$

for any $f^{(N)} \equiv f_1 \otimes \cdots \otimes f_N$, $g^{(N)} \equiv g_1 \otimes \cdots \otimes g_N \in \mathfrak{h}^{\otimes N}$ and extension by linearity.

The Fock space $\mathcal{F}$ is defined as the direct sum of all N-particle Hilbert spaces,

$$\mathcal{F} \equiv \mathcal{F}[\mathfrak{h}] := \bigoplus_{N=0}^{\infty} \mathfrak{h}^{\otimes N}.$$

Here by convention $\mathfrak{h}^{\otimes 0} := \mathbb{C}$. For $\mathfrak{h}^{\otimes 0}$ we set $\left\langle f^{(0)}, g^{(0)} \right\rangle_{\mathfrak{h}^{\otimes 0}} := \overline{f}^{(0)} g^{(0)}$ for $f^{(0)}, g^{(0)} \in \mathfrak{h}^{\otimes 0}$. Any vector $\Psi \in \mathcal{F}$ can be written as a sequence of N-particle wave functions $f^{(N)} \in \mathfrak{h}^{\otimes N}$:

$$\Psi = \left(f^{(N)} \right)_{N=0}^{\infty}.$$

The vacuum vector $\Omega := (1, 0, 0, \dots) \in \mathcal{F}$ is considered as the basis vector of $\mathfrak{h}^{\otimes 0}$. With the inner product $\langle \cdot, \cdot \rangle_{\mathcal{F}} : \mathcal{F} \times \mathcal{F} \to \mathbb{C}$ defined by

$$\langle \Psi, \Phi \rangle_{\mathcal{F}} := \sum_{N=0}^{\infty} \left\langle f^{(N)}, g^{(N)} \right\rangle_{\mathfrak{h}^{\otimes N}}$$

for any $\Psi \equiv \left(f^{(N)} \right)_{N=0}^{\infty}$ and $\Phi \equiv \left(g^{(N)} \right)_{N=0}^{\infty} \in \mathcal{F}$ the Fock space is a Hilbert space.

The particle number operator is defined as

$$\widehat{\mathbb{N}} := \bigoplus_{N=0}^{\infty} N \mathbb{1}_{\mathfrak{h}^{\otimes N}}.$$

For any bounded operator $C \in \mathcal{B}(\mathfrak{h})$ $\Gamma(C) := \bigoplus_{N=0}^{\infty} C^{\otimes N}$ is an operator on $\mathcal{F}$. In particular, $\Gamma(C)$ is trace class, $\Gamma(C) \in \mathcal{L}^1(\mathcal{F})$, if $C \in \mathcal{L}^1(\mathfrak{h})$ and for bosons additionally $\|C\|_{\mathcal{B}(\mathfrak{h})} \leq 1$.

A detailed description of the Fock representation can be found for instance in [BR86, BR79, BR81, Sol07, Thi08].

2.1 Bosons

The boson Fock space is the symmetric subspace of the Fock space $\mathcal{F}$, i.e.,

$$\mathcal{F}^{+} \equiv \mathcal{F}^{+}[\mathfrak{h}] := S \bigoplus_{N=0}^{\infty} \mathfrak{h}^{\otimes N}.$$

Here the symmetrization operator $S \in \mathcal{B}(\mathcal{F})$ is defined by

$$S \left(f^{(N)} \right)_{N=0}^{\infty} := \left(\frac{1}{N!} \sum_{\pi \in \mathfrak{S}_N} \bigotimes_{k=1}^{N} f^{(N)}_{\pi(k)} \right)_{N=0}^{\infty}$$

with $f^{(N)} = f_1^{(N)} \otimes \cdots \otimes f_N^{(N)} \in \mathfrak{h}^{\otimes N}$ for any $N \in \mathbb{N}$ where $\mathfrak{S}_N$ denotes the symmetric group with permutations π of N elements.

Definition 3.1. For any $f \in \mathfrak{h}$ the boson creation and annihilation operators are denoted by $a^*(f)$ and $a(f)$, respectively. Their domain, which lies dense in $\mathcal{F}^+$, is

$$\mathcal{D}(\widehat{\mathbb{N}}^{\frac{1}{2}}) \cap \mathcal{F}^+ = \left\{ \Psi \equiv \left(f^{(N)}\right)_{N=0}^{\infty} \in \mathcal{F}^+ \middle| \sum_{N=0}^{\infty} (N+1) \left\| f^{(N)} \right\|^2 < \infty \right\}.$$

A complete characterization of a^* and a is given by the properties

$$a(f)\Omega = 0, \quad a^*(f)\Omega = f,$$

and the canonical commutation relations (CCR)

$$[a^*(f), a^*(g)] = 0, \quad [a(f), a(g)] = 0, \text{ and}$$
$$[a(f), a^*(g)] = \langle f, g \rangle \, \mathbb{1}_{\mathcal{F}^+}$$

for any $f, g \in \mathfrak{h}$ where $\mathbb{1}_{\mathcal{F}^+} \in \mathcal{B}(\mathcal{F})$ is the identity operator restricted the boson Fock space and $[A, B] := AB - BA$ the commutator.

The creation operator $a^*(f)$ is linear in f while the annihilation operator $a(f)$ is antilinear. Furthermore the creation and annihilation operators are adjoints of each other: $a^*(f) = (a(f))^*$. Henceforth we use the abbreviations $a_k^* \equiv a^*(\varphi_k)$ and $a_k \equiv a(\varphi_k)$ for a fixed, but arbitrary orthonormal basis (ONB) $\{\varphi_k\}_{k=1}^{\infty}$ of $\mathfrak{h}$.

For any ONB $\{\varphi_k\}_{k=1}^{\infty}$ of $\mathfrak{h}$ the particle number operator reads

$$\widehat{\mathbb{N}} = \sum_{k=1}^{\infty} a_k^* a_k$$

as a quadratic form on $\mathcal{F}^+$.

Unlike the fermion case the space generated by all boson creation and annihilation operators cannot be used to define a C^*-algebra. To this end we introduce the Weyl operators and construct the CCR algebra. For a detailed survey see, e.g., [BR81].

For every $f \in \mathfrak{h}$ we define the field operator $\Phi(f) : \mathcal{D}(\Phi(f)) \subseteq \mathcal{F}^+ \to \mathcal{F}^+$ by

$$\Phi(f) := \frac{1}{\sqrt{2}} \left(a^*(f) + a(f)\right).$$

The field operator is essentially selfadjoint on $\mathcal{F}^+$. Therefore its closure is selfadjoint and we denote it by $\Phi(f)$ as well.

Definition 3.2. For every $f \in \mathfrak{h}$ the unitary transformation $\mathbb{W}(f) : \mathcal{F}^+ \to \mathcal{F}^+$, called Weyl operator, is defined by

$$\mathbb{W}(f) := \exp\left(\mathrm{i}\Phi(f)\right).$$

The Weyl operators satisfy $\mathbb{W}(f)^* = \mathbb{W}(-f)$ and the Weyl commutation relations

$$\mathbb{W}(f)\,\mathbb{W}(g) = \mathrm{e}^{-\frac{\mathrm{i}}{2}\,\mathrm{Im}\langle f,g\rangle_{\mathfrak{h}}}\,\mathbb{W}(f+g)$$

for any $f, g \in \mathfrak{h}$. The commutator of two Weyl operators is completely determined by the Weyl commutation relations. Furthermore, we have $\mathbb{W}(0) = \mathbb{1}_{\mathcal{F}^+}$.

A given field operator $\Phi(f)$ with $f \in \mathfrak{h}$ is transformed by the Weyl operator $\mathbb{W}(g)$ with $g \in \mathfrak{h}$ as

$$\mathbb{W}(g)\Phi(f)\mathbb{W}(g)^* = \Phi(f) - \mathrm{Im}\,\langle g, f\rangle_{\mathfrak{h}}\,\mathbb{1}_{\mathcal{F}^+}.$$

Hence, $\mathbb{W}_g \equiv \mathbb{W}(\mathrm{i}\sqrt{2}g)$ defines a unitary transformation, called Weyl transformation, for any $g \in \mathfrak{h}$. For any $f \in \mathfrak{h}$ this transformation yields

$$\mathbb{W}_g a^*(f)\mathbb{W}_g^* = a^*(f) + \langle g, f\rangle_{\mathfrak{h}}\,\mathbb{1}_{\mathcal{F}^+} \text{ and}$$
$$\mathbb{W}_g a(f)\mathbb{W}_g^* = a(f) + \langle f, g\rangle_{\mathfrak{h}}\,\mathbb{1}_{\mathcal{F}^+}.$$

Definition 3.3. The C^*-algebra $\mathcal{W}$ generated by $\left\{\mathbb{W}(f)\middle| f \in \mathfrak{h}\right\}$ is called Weyl algebra or CCR algebra.

This algebra is unique up to $*$-automorphisms (Cf. Theorem 5.2.8. of [BR81]).

2.1.1 Boson Bogoliubov Transformation

Remark 3.4. The following definition of the Bogoliubov transformation depends on the choice of the ONB $\{\varphi_k\}_{k=1}^{\infty}$ of $\mathfrak{h}$ since the complex conjugate of a function $f \in \mathfrak{h}$, that is given by $f = \sum_{k=1}^{\infty} \mu_k \varphi_k$ with some $\mu_k \in \mathbb{C}, k \in \mathbb{N}$, is defined by

$$\overline{f} := \sum_{k=1}^{\infty} \overline{\mu}_k \varphi_k. \tag{3.12}$$

Furthermore, we define for any operator A the complex conjugate operator $\overline{A}$ by

$$\langle f, \overline{A}g\rangle := \overline{\left\langle \overline{f}, A\overline{g}\right\rangle}. \tag{3.13}$$

We emphasize that there is also a formulation to obtain a basis independent definition of the Bogoliubov transformation, e.g., in [Sol07, Nam11]. There the underlying space is $\mathfrak{h} \oplus \mathfrak{h}^*$ instead of $\mathfrak{h} \oplus \mathfrak{h}$ and an antilinear map $J : \mathfrak{h} \to \mathfrak{h}^*$, defined by $Jg(f) := \langle g, f\rangle_{\mathfrak{h}}$ for any $f, g \in \mathfrak{h}$, and its inverse $J^* : \mathfrak{h}^* \to \mathfrak{h}$ are required. Then the second component of a vector $f \oplus g \in \mathfrak{h} \oplus \mathfrak{h}$ is replaced by $Jg \in \mathfrak{h}^*$ such that $f \oplus Jg \in \mathfrak{h} \oplus \mathfrak{h}^*$. The new vector is antilinear in the second component. This supersedes the definition of the complex conjugate of a function. Furthermore some operators map from $\mathfrak{h}^*$ to $\mathfrak{h}$ or vice versa, e.g., $v : \mathfrak{h} \to \mathfrak{h}^*$. Then, for instance, $\overline{v}$ and $\overline{u}$ of the following definition are replaced by the maps $v : \mathfrak{h} \to \mathfrak{h}^*$ and $JuJ^* : \mathfrak{h}^* \to \mathfrak{h}^*$, respectively.

For any linear operator A the transpose is defined as $A^T := \overline{A}^* = \overline{A^*}$. Now we are prepared to define a boson Bogoliubov transformation.

Definition 3.5. A linear map $U = \left(\begin{smallmatrix} u & v \\ \bar{v} & \bar{u} \end{smallmatrix}\right) : \mathfrak{h} \oplus \mathfrak{h} \to \mathfrak{h} \oplus \mathfrak{h}$ is called boson Bogoliubov transformation if the linear operators $u : \mathfrak{h} \to \mathfrak{h}$ and $v : \mathfrak{h} \to \mathfrak{h}$ fulfill

$$uu^* - vv^* = \mathbb{1}_{\mathfrak{h}}, \quad u^*u - v^T\bar{v} = \mathbb{1}_{\mathfrak{h}}, \tag{3.14a}$$

$$u^*v - v^T\bar{u} = 0, \quad uv^T - vu^T = 0. \tag{3.14b}$$

Remark 3.6. Eqs. (3.14a,b) on u and v are equivalent to stating

$$U^*\mathcal{S}U = \mathcal{S} \quad \text{and} \quad U\mathcal{S}U^* = \mathcal{S}$$

with

$$\mathcal{S} := \begin{pmatrix} \mathbb{1}_{\mathfrak{h}} & 0 \\ 0 & -\mathbb{1}_{\mathfrak{h}} \end{pmatrix}.$$

As can be easily deduced from Remark 3.6, any boson Bogoliubov transformation U is invertible. The inverse is given by the Bogoliubov transformation

$$U^{-1} = \mathcal{S}U^*\mathcal{S}.$$

Lemma 3.7. *Let $U = \left(\begin{smallmatrix} u & v \\ \bar{v} & \bar{u} \end{smallmatrix}\right) : \mathfrak{h} \oplus \mathfrak{h} \to \mathfrak{h} \oplus \mathfrak{h}$ be a boson Bogoliubov transformation. There is a unitary transformation $\mathbb{U}_U : \mathcal{F}^+ \to \mathcal{F}^+$ such that*

$$\mathbb{U}_U \left[a^*(f) + a(\bar{g})\right] \mathbb{U}_U^* = a^*(uf + vg) + a(v\bar{f} + u\bar{g})$$

for all $f, g \in \mathfrak{h}$ if and only if v is Hilbert–Schmidt. We call $\mathbb{U}_U$ unitary representation or implementation of U on $\mathcal{F}^+$.

The condition that v is Hilbert–Schmidt is named after Shale and Stinespring [SS65].

2.1.2 States and Density Matrices

After introducing the CCR algebra and the Bogoliubov transformation, we are prepared to define states, certain subclasses of states, and afterwards density matrices.

Definition 3.8. A continuous linear functional $\omega \in \mathcal{W}^*$ on the CCR algebra $\mathcal{W}$ is called a state if it is normalized and positive, i.e., $\omega(\mathbb{1}_{\mathcal{F}^+}) = 1$ and $\omega(A) \geq 0$ for all positive semi-definite operators $A \in \mathcal{W}$.

Since the boson creation and annihilation operators are not in $\mathcal{W}$, their expectation values are not well-defined for all states. In order to find well-defined expressions for these expectation values, we first restrict ourselves to specific states and then extend the domain for these states appropriately.

Let $\mathbb{W}(f)$ denote a Weyl operator for any $f \in \mathfrak{h}$ and let ω be a state. We assume that the map $T_f : \mathbb{R} \to \mathbb{C}$, $t \mapsto \omega\big(\mathbb{W}(tf)\big)$, is four times continuously differentiable for all $f \in \mathfrak{h}$, shortly $T_f \in \mathcal{C}^4(\mathbb{R};\mathbb{C})$. This assumption provides the definition of the expectation value of a single creation or annihilation operator and of the particle number operator. For instance, we have

$$\omega\big(\Phi(f)\big) := \frac{\mathrm{d}}{\mathrm{d}t}\omega\big(\mathbb{W}(tf)\big)\Big|_{t=0} < \infty$$

for any $f \in \mathfrak{h}$ and hence by linearity of ω

$$\omega\big(a(f)\big) = \frac{1}{\sqrt{2}}\left[\omega\big(\Phi(f)\big) + \mathrm{i}\omega\big(\Phi(\mathrm{i}f)\big)\right].$$

Analogously we give a meaning to

$$\omega\big(a^*(f)\big), \quad \omega\big(e(f)\,e(g)\big), \quad \text{and} \quad \omega\big(e(f_1)\,e(f_2)\,e(g_2)\,e(g_1)\big)$$

for $f, g, f_1, f_2, g_1, g_2 \in \mathfrak{h}$ due to $T_f \in \mathcal{C}^4(\mathbb{R};\mathbb{C})$. Here e denotes either the creation operator a^* or the annihilation operator a. Thus the expectation value in this state ω can be defined not only for elements of the CCR-algebra, but also for polynomials of degree 4 in creation and annihilation operators. In order to exemplify such polynomials, we note that, e.g., a general polynomial of degree 2 can be written as

$$\mathcal{P}_2 := \sum_{k,l=1}^{N}\left[\alpha_{kl}a_k^*a_l + \beta_{kl}a_k^*a_l^* + \epsilon_{kl}a_ka_l\right] + \sum_{k=1}^{N}\left[\zeta_k a_k^* + \xi_k a_k\right] + \mu$$

with an ONB $\{\varphi_k\}_{k=1}^{\infty}$ of $\mathfrak{h}$, some $N \in \mathbb{N}$, and $\alpha_{kl}, \beta_{kl}, \epsilon_{kl}, \zeta_k, \xi_k, \mu \in \mathbb{C}$ for $1 \leq k, l \leq N$. In Appendix B we show how to simplify such polynomials of degree 2. In particular, we find conditions for a diagonalization of the quadratic and (at least partial) cancellation of the linear part using a Bogoliubov–Weyl transformation.

Definition 3.9. We denote the closure of the indicated extension to the polynomials of degree 4 in creation and annihilation operators by $\mathcal{A}^+$.

For any ONB $\{\varphi_k\}_{k=1}^{\infty}$ of $\mathfrak{h}$ the monotonously increasing sequence of the polynomials $\widehat{\mathbb{N}}_N := \sum_{k=1}^{N} a_k^* a_k$ with $N \in \mathbb{N}$ converges strongly to the particle number operator $\widehat{\mathbb{N}}$ on

$$\mathcal{D}(\widehat{\mathbb{N}}) \cap \mathcal{F}^+ = \left\{\Psi \equiv \left(f^{(N)}\right)_{N=0}^{\infty} \in \mathcal{F}^+ \,\middle|\, \sum_{N=0}^{\infty}(N+1)^2\left\|f^{(N)}\right\|^2 < \infty\right\}.$$

Definition 3.10. Let ω be a state. If $T_f \in \mathcal{C}^4(\mathbb{R};\mathbb{C})$ for any $f \in \mathfrak{h}$ and $\omega\big(\widehat{\mathbb{N}}^2\big) := \lim_{N\to\infty}\omega\big(\widehat{\mathbb{N}}_N^2\big) < \infty$, we write $\omega \in \mathcal{Z}^+$. For any $N \in \mathbb{N}$, we denote the subset of all N-particle states, i.e., states satisfying $\omega\big(\widehat{\mathbb{N}}\big) = N$, by $\mathcal{Z}_N^+$.

For any $\omega \in \mathcal{Z}^+$ the Cauchy–Schwarz inequality yields

$$\omega\big(\widehat{\mathbb{N}}\big) \leq \sqrt{\omega\big(\widehat{\mathbb{N}}^2\big)} < \infty.$$

Definition 3.11. A state $\omega \in \mathcal{Z}^+$ is called pure if there is a $\Psi \in \mathcal{F}^+$ such that for any $A \in \mathcal{A}^+$

$$\omega(A) = \langle \Psi, A\Psi \rangle_{\mathcal{F}} .$$

Definition 3.12. A centered state is a state $\omega \in \mathcal{Z}^+$ with

$$\omega\big(a^*(f)\big) = 0 \tag{3.15}$$

for any $f \in \mathfrak{h}$. We denote the set of all centered states by $\mathcal{Z}^+_{\mathrm{cen}}$.

As follows from (3.15), we also have $\omega\big(a(f)\big) = 0$ for $\omega \in \mathcal{Z}^+_{\mathrm{cen}}$.

Definition 3.13. A state $\omega \in \mathcal{Z}^+$ is called quasifree, shortly $\omega \in \mathcal{Z}^+_{\mathrm{qf}}$, if there is a positive semi-definite operator h_ω on $\mathfrak{h}$ and $f_\omega \in \mathfrak{h}$ such that for every $f \in \mathfrak{h}$

$$\omega(\mathbb{W}_f) = \exp\Big(-2\mathrm{i}\, \langle f_\omega, f\rangle_{\mathfrak{h}} - \langle f, (\mathbb{1}_{\mathfrak{h}} + h_\omega)\, f\rangle_{\mathfrak{h}}\Big) .$$

The subset of pure quasifree states is denoted by $\mathcal{Z}^+_{\mathrm{pqf}}$.

The sets $\mathcal{Z}^+_{\mathrm{qf}}$ and $\mathcal{Z}^+_{\mathrm{pqf}}$ are invariant under Bogoliubov and Weyl transformations, i.e., the transform of a (pure) quasifree state is (pure) quasifree as well.

Remark 3.14. Any centered quasifree state $\omega \in \mathcal{Z}^+_{\mathrm{cqf}} := \mathcal{Z}^+_{\mathrm{cen}} \cap \mathcal{Z}^+_{\mathrm{qf}}$ fulfills Wick's Theorem (in a simplified form), namely,

$$\begin{aligned} &\omega(e_1 e_2 \cdots e_{2n-1}) = 0 \quad \text{and} \\ &\omega(e_1 e_2 \cdots e_{2n}) = \sum_{\pi} \omega(e_{\pi(1)} e_{\pi(2)}) \cdots \omega(e_{\pi(2n-1)} e_{\pi(2n)}) \end{aligned}$$

for every $n \in \mathbb{N}$ where e_i denotes either the creation operator a_i^* or the annihilation operator a_i for every $i \in \{1, 2, \ldots, 2n\}$. The sum is taken over all permutations $\pi \in \mathfrak{S}_{2n}$ satisfying

$$\pi(1) < \pi(3) < \cdots < \pi(2n-1) \text{ and } \pi(2k-1) < \pi(2k)$$

for every $k \in \{1, 2, \ldots, n\}$. Note that for non-centered quasifree states a more complicated version of Wick's Theorem holds which we omit here and refer the reader to, e.g., [BR86].

Definition 3.15. We say that a state $\omega \in \mathcal{Z}^+$ is coherent, $\omega \in \mathcal{Z}^+_{\mathrm{coh}}$, if there is an $f \in \mathfrak{h}$ such that for all $A \in \mathcal{A}^+$

$$\omega(A) = \Big\langle \Omega, \mathbb{W}_f A \mathbb{W}_f^* \Omega \Big\rangle_{\mathcal{F}} .$$

In particular we have

$$\mathcal{Z}^+_{\mathrm{cqf}} \subsetneq \mathcal{Z}^+_{\mathrm{qf}} \quad \text{and} \quad \mathcal{Z}^+_{\mathrm{coh}} \subsetneq \mathcal{Z}^+_{\mathrm{pqf}} \subsetneq \mathcal{Z}^+_{\mathrm{qf}} .$$

Definition 3.16. We call a positive semi-definite operator $\rho \in \mathcal{L}^1(\mathcal{F}^+)$ with $\mathrm{tr}_{\mathcal{F}^+}(\rho) = 1$ a density matrix.

For a density matrix $\rho \in \mathcal{L}^1(\mathcal{F}^+)$ the map

$$\mathcal{A}^+ \to \mathbb{C},\ A \mapsto \mathrm{tr}_{\mathcal{F}^+}\big(\rho^{\frac{1}{2}} A \rho^{\frac{1}{2}}\big)$$

defines a state. In particular for every state $\omega \in \mathcal{Z}^+$ there is a density matrix ρ with $\mathrm{tr}_{\mathcal{F}^+}\big(\rho^{\frac{1}{2}} A \rho^{\frac{1}{2}}\big) = \omega(A)$ for all $A \in \mathcal{A}^+$. Therefore the notions of pureness, quasifreeness etc. can be transferred to the corresponding density matrix.

2.1.3 One- and Two-Particle Density Matrices and Representability

For systems with a one-particle part and pair-interactions the formulation of the variational problem can be reduced by the notion of one- and two-particle density matrices.

Definition 3.17. For any state $\omega \in \mathcal{Z}^+$ the corresponding (boson) one-particle density matrix (1-pdm) $\gamma_\omega : \mathfrak{h} \to \mathfrak{h}$ is defined by its matrix elements

$$\langle f, \gamma_\omega g \rangle_{\mathfrak{h}} := \omega\big(a^*(g)\, a(f)\big) \tag{3.16}$$

for every $f, g \in \mathfrak{h}$.

Since any state is positive, we have

$$\langle f, \gamma_\omega f \rangle_{\mathfrak{h}} = \omega\big(a^*(f)\, a(f)\big) \geq 0$$

for any $f \in \mathfrak{h}$. Hence the 1-pdm is a selfadjoint and positive semi-definite operator. Moreover $\gamma_\omega \in \mathcal{L}^1(\mathfrak{h})$ due to

$$\mathrm{tr}_{\mathfrak{h}}\left(\gamma_\omega\right) = \sum_{k=1}^{\infty} \langle \varphi_k, \gamma_\omega \varphi_k \rangle_{\mathfrak{h}} = \omega\Big(\sum_{k=1}^{\infty} a_k^* a_k\Big) = \omega\big(\widehat{\mathbb{N}}\big) < \infty.$$

Definition 3.18. The (boson) two-particle density matrix (2-pdm) $\Gamma_\omega : \mathfrak{h} \otimes \mathfrak{h} \to \mathfrak{h} \otimes \mathfrak{h}$ of a state $\omega \in \mathcal{Z}^+$ is defined by

$$\langle f_1 \otimes f_2, \Gamma_\omega\left(g_1 \otimes g_2\right) \rangle := \omega\big(a^*(g_2)\, a^*(g_1)\, a(f_1)\, a(f_2)\big)$$

for any $f_1, f_2, g_1, g_2 \in \mathfrak{h}$.

The 2-pdm is a positive semi-definite trace class operator since

$$\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\Gamma_\omega\right) = \omega\big(\widehat{\mathbb{N}}^2 - \widehat{\mathbb{N}}\big) < \infty$$

and for any $\psi \equiv \sum_{k,l=1}^{\infty} \mu_{kl} (\varphi_k \otimes \varphi_l) \in \mathfrak{h} \otimes \mathfrak{h}$, $\mu_{kl} \in \mathbb{C}$

$$\langle \psi, \Gamma_\omega \psi \rangle_{\mathfrak{h}\otimes\mathfrak{h}} = \sum_{i,j,k,l=1}^{\infty} \mu_{kl} \overline{\mu}_{ij} \omega\big(a_k^* a_l^* a_j a_i\big) = \omega\big(PP^*\big) \geq 0$$

where $P := \sum_{k,l=1}^{\infty} \mu_{kl} a_k^* a_l^*$. Furthermore the 2-pdm is symmetric, i.e., $\Gamma_\omega \operatorname{Ex} = \operatorname{Ex} \Gamma_\omega = \Gamma_\omega$. Here the exchange operator $\operatorname{Ex} : \mathfrak{h} \otimes \mathfrak{h} \to \mathfrak{h} \otimes \mathfrak{h}$ is the linear map defined by

$$\operatorname{Ex}(f \otimes g) := g \otimes f$$

for any $f, g \in \mathfrak{h}$. Summarizing the basic properties of the 1- and 2-pdm, we introduce the notions of admissibility and representability.

Definition 3.19. We call a pair (γ, Γ) of operators on $\mathfrak{h} \times (\mathfrak{h} \otimes \mathfrak{h})$ admissible if

(i) $\Gamma \in \mathcal{L}^1(\mathfrak{h} \otimes \mathfrak{h})$ is symmetric, i.e., $\operatorname{Ex}\Gamma = \Gamma \operatorname{Ex} = \Gamma$, and selfadjoint, and

(ii) $\gamma \in \mathcal{L}^1(\mathfrak{h})$ with $\operatorname{tr}_{\mathfrak{h}}(\gamma) = \omega(\widehat{\mathbb{N}})$ is selfadjoint and positive semi-definite.

Definition 3.20. We say that the pair (γ, Γ) of operators on $\mathfrak{h}$ and $\mathfrak{h} \otimes \mathfrak{h}$, respectively, is representable if there is a state $\omega \in \mathcal{Z}^+$ with $\gamma_\omega = \gamma$ and $\Gamma_\omega = \Gamma$. Necessary conditions on the pair (γ, Γ) to be representable are called representability conditions.

Every representable pair (γ, Γ) is in particular admissible. Note that in the literature also the term "N-representability" appears which is obtained by replacing $\mathcal{Z}^+$ by $\mathcal{Z}_N^+$ in the previous definition, i.e., if we assume (γ, Γ) to be the 1- and 2-pdm of a N-particle state.

2.1.4 Generalized One- and Two-Particle Density Matrices for Bosons

In [BLS94] a generalized one-particle density matrix is defined for fermions on the space $\mathfrak{h} \oplus \mathfrak{h}$. We provide a definition of the generalized 1-pdm for bosons and then further generalize the one- and the two-particle density matrices. Again the subsequent definitions depend on the choice of the ONB of $\mathfrak{h}$ since we use complex conjugates of functions, as well as operators as explained in Remark 3.4. We refer the reader to [Sol07] for a basis independent formulation.

Definition 3.21. For any state $\omega \in \mathcal{Z}^+$ the generalized one-particle density matrix $\widetilde{\gamma}_\omega$ is an operator on $\mathfrak{h} \oplus \mathfrak{h}$ defined by

$$\langle (f_1 \oplus f_2), \widetilde{\gamma}_\omega (g_1 \oplus g_2) \rangle_{\mathfrak{h}\oplus\mathfrak{h}} := \omega\Big([a^*(g_1) + a(\overline{g}_2)] \Big[a(f_1) + a^*(\overline{f}_2)\Big] \Big) \tag{3.17}$$

for $f_1, f_2, g_1, g_2 \in \mathfrak{h}$.

Remark 3.22. Defining

$$\alpha_\omega^* : \mathfrak{h} \to \mathfrak{h}, \ \langle f, \alpha_\omega^* g \rangle_{\mathfrak{h}} := \omega\big(a^*(g)\, a^*(\overline{f})\big), \tag{3.18}$$

we are able to write the generalized 1-pdm as

$$\widetilde{\gamma}_\omega = \begin{pmatrix} \gamma_\omega & \alpha_\omega \\ \alpha_\omega^* & \mathbb{1}_{\mathfrak{h}} + \overline{\gamma}_\omega \end{pmatrix},$$

a matrix with operator-valued entries. The 1-pdm γ_ω is selfadjoint and α_ω symmetric, i.e., $\alpha_\omega^T = \alpha_\omega$ for its transpose $\alpha_\omega^T := \overline{\alpha_\omega^*}$.

Lemma 3.23. *For any $\omega \in \mathcal{Z}^+$ the generalized one-particle density matrix $\widetilde{\gamma}_\omega$ as defined by (3.17) is a positive semi-definite operator on $\mathfrak{h} \oplus \mathfrak{h}$. In particular it is selfadjoint.*

Proof. By setting $g_1 = f_1$ and $g_2 = f_2$ the assertion is a direct consequence of (3.17) and the positivity of the corresponding state. □

Therefore the boson 1-pdm γ is positive semi-definite, too. Unlike the fermion case the boson 1-pdm is not bounded above by $\mathbb{1}_\mathfrak{h}$.

So far the definitions and statements are well established and can be found, for example, in [Nam11], in [Sol07] for both particle types, and, in a version for fermions, in [BLS94].

Lemma 3.24. *Let $\omega \in \mathcal{Z}^+$ be a state and $\widetilde{\gamma} : \mathfrak{h} \oplus \mathfrak{h} \to \mathfrak{h} \oplus \mathfrak{h}$ its generalized one-particle density matrix. For a boson Bogoliubov transformation $U : \mathfrak{h} \oplus \mathfrak{h} \to \mathfrak{h} \oplus \mathfrak{h}$ with unitary representation $\mathbb{U}_U : \mathcal{F}^+ \to \mathcal{F}^+$ define a state ω_U by $\omega_U(A) := \omega(\mathbb{U}_U A \mathbb{U}_U^*)$ for any $A \in \mathcal{A}^+$. Then the generalized one-particle density matrix $\widetilde{\gamma}_U$ of the state ω_U is given by*

$$\widetilde{\gamma}_U = U^* \widetilde{\gamma} U. \tag{3.19}$$

Furthermore $\widetilde{\gamma}\mathcal{S}\widetilde{\gamma} = -\widetilde{\gamma}$ implies $\widetilde{\gamma}_U \mathcal{S} \widetilde{\gamma}_U = -\widetilde{\gamma}_U$.

Proof. We consider the matrix elements of $\widetilde{\gamma}_U$. For the first assertion we obtain

$$\begin{aligned}
&\langle (f_1 \oplus f_2), \widetilde{\gamma}_U (g_1 \oplus g_2) \rangle_{\mathfrak{h}\oplus\mathfrak{h}} \\
&\qquad = \omega\Big(\mathbb{U}_U \left[a^*(g_1) + a(\overline{g}_2) \right] \mathbb{U}_U^* \mathbb{U}_U \left[a(f_1) + a^*(\overline{f}_2) \right] \mathbb{U}_U^* \Big) \\
&\qquad = \omega\big(\left[a^*(ug_1 + vg_2) + a(u\overline{g}_2 + v\overline{g}_1) \right] \\
&\qquad\qquad \times \left[a(uf_1 + vf_2) + a^*(u\overline{f}_2 + v\overline{f}_1) \right] \big) \\
&\qquad = \langle U (f_1 \oplus f_2), \widetilde{\gamma} U (g_1 \oplus g_2) \rangle_{\mathfrak{h}\oplus\mathfrak{h}}
\end{aligned}$$

for any $f_1, f_2, g_1, g_2 \in \mathfrak{h}$. Thus, (3.19) holds.

The second assertion follows from (3.19) and $U\mathcal{S}U^* = \mathcal{S}$:

$$\widetilde{\gamma}_U \mathcal{S} \widetilde{\gamma}_U = U^* \widetilde{\gamma} U \mathcal{S} U^* \widetilde{\gamma} U = U^* \widetilde{\gamma} \mathcal{S} \widetilde{\gamma} U = -U^* \widetilde{\gamma} U = -\widetilde{\gamma}_U$$

which completes the proof. □

In the following we give a further generalization of the 1-pdm on the space $\mathfrak{H}_{\text{gen}} := \mathfrak{h} \oplus \mathfrak{h} \oplus \mathbb{C}$.

Definition 3.25. For any state $\omega \in \mathcal{Z}^+$ the further generalized one-particle density matrix $\widehat{\gamma}_\omega : \mathfrak{H}_{\text{gen}} \to \mathfrak{H}_{\text{gen}}$ is defined by

$$\langle G, \widehat{\gamma}_\omega F \rangle_{\mathfrak{H}_{\text{gen}}} := \omega\big(\left[a^*(f_1) + a(\overline{f}_2) + \mu \right] \left[a(g_1) + a^*(\overline{g}_2) + \overline{\nu} \right] \big) \tag{3.20}$$

for $F \equiv f_1 \oplus f_2 \oplus \mu$ and $G \equiv g_1 \oplus g_2 \oplus \nu \in \mathfrak{H}_{\text{gen}}$.

Remark 3.26. We rewrite the further generalized 1-pdm $\widehat{\gamma}_\omega$ as a (3×3)-matrix:

$$\widehat{\gamma}_\omega = \begin{pmatrix} \gamma_\omega & \alpha_\omega & b_\omega \\ \alpha_\omega^* & \mathbb{1}_{\mathfrak{h}} + \overline{\gamma}_\omega & \overline{b}_\omega \\ b_\omega^* & \overline{b}_\omega^* & 1 \end{pmatrix}. \tag{3.21}$$

Here the first moment $b_\omega \in \mathfrak{h}$ and its dual element $b_\omega^* \in \mathfrak{h}^*$ are given by

$$\langle g, b_\omega \rangle_{\mathfrak{h}} := \omega\big(a(g)\big) \quad \text{and} \quad b_\omega^* \cdot g \equiv \langle b_\omega, g \rangle_{\mathfrak{h}} = \omega\big(a^*(g)\big) \tag{3.22}$$

for every $g \in \mathfrak{h}$. For the complex conjugate $\overline{b}_\omega$ of the wave function $b_\omega \in \mathfrak{h}$ we have $\left\langle g, \overline{b}_\omega \right\rangle_{\mathfrak{h}} = \overline{\langle \overline{g}, b_\omega \rangle_{\mathfrak{h}}} = \overline{\omega\big(a(\overline{g})\big)} = \omega\big(a^*(\overline{g})\big)$.

Proposition 3.27. *The further generalized one-particle density matrix is positive semi-definite and selfadjoint.*

Proof. The selfadjointness is a direct consequence of (3.21). By setting $F = G$ in (3.20) $\widehat{\gamma} \geq 0$ follows from the positivity of the state ω. ☐

Lemma 3.28. *Let* $\widehat{\gamma} = \begin{pmatrix} \gamma & \alpha & b \\ \alpha^* & \mathbb{1}_{\mathfrak{h}} + \overline{\gamma} & \overline{b} \\ b^* & \overline{b}^* & 1 \end{pmatrix} : \mathfrak{h} \oplus \mathfrak{h} \oplus \mathbb{C} \to \mathfrak{h} \oplus \mathfrak{h} \oplus \mathbb{C}$ *be a positive semi-definite operator with* $b \in \mathfrak{h}$, $\gamma \in \mathcal{L}^1(\mathfrak{h})$, *and* $\alpha \in \mathcal{L}^2(\mathfrak{h})$. *Then there is a unique quasifree state* ω *that has* $\widehat{\gamma}$ *as its further generalized one-particle density matrix.*
In particular for any positive semi-definite operator $\widetilde{\gamma} = \begin{pmatrix} \gamma & \alpha \\ \alpha^* & \mathbb{1}_{\mathfrak{h}} + \overline{\gamma} \end{pmatrix} : \mathfrak{h} \oplus \mathfrak{h} \to \mathfrak{h} \oplus \mathfrak{h}$ *with* $\gamma \in \mathcal{L}^1(\mathfrak{h})$ *and* $\alpha \in \mathcal{L}^2(\mathfrak{h})$ *there is a state* $\omega \in \mathcal{Z}_{\mathrm{cqf}}^+$ *with* $\widetilde{\gamma} = \widetilde{\gamma}_\omega$.

Proof. The second part is a consequence of Theorem 11.4 in [Sol07] or Theorem 1.6 (i) in [Nam11]. The first part follows from the second part due to the fact that a non-centered state with first moment $b \in \mathfrak{h}$ is completely characterized by a Weyl operator $\mathbb{W}_b$ and the centered state ω_0 defined by $\omega_0(A) := \omega(\mathbb{W}_b^* A \mathbb{W}_b)$ for any $A \in \mathcal{A}^-$. ☐

Analogously we define a generalized two-particle density matrix $\widehat{\Gamma}$ on

$$\mathfrak{H}_{\mathrm{sim}} := \left(\bigoplus_{n=1}^{4} \mathfrak{h} \otimes \mathfrak{h} \right) \oplus \left(\bigoplus_{n=1}^{2} \mathfrak{h} \right) \oplus \mathbb{C}.$$

Technically the generalized 2-pdm should be defined on

$$\mathfrak{H}_{\mathrm{gen}} \otimes \mathfrak{H}_{\mathrm{gen}} \cong \left(\bigoplus_{n=1}^{4} \mathfrak{h} \otimes \mathfrak{h} \right) \oplus \left(\bigoplus_{n=1}^{4} \mathfrak{h} \right) \oplus \mathbb{C}.$$

It suffices, however, to consider $\mathfrak{H}_{\mathrm{sim}}$ since for any polynomial of degree 1 in annihilation and creation operators there are an ONB $\{\varphi_k\}_{k=1}^\infty$ of $\mathfrak{h}$, an $N \in \mathbb{N}$, and coefficients $\mu_k, \nu_k, \sigma_k \tau_k, \tilde{\mu}_k, \tilde{\nu}_k \in \mathbb{C}, k = 1, \ldots, N$, such that

$$\sum_{k=1}^{N} \left(\mu_k a_k^* + \nu_k a_k + \overline{\sigma}_k a_k + \overline{\tau}_k a_k^* \right) = \sum_{k=1}^{N} \left(\tilde{\mu}_k a_k^* + \tilde{\nu}_k a_k \right).$$

Let $M \in \mathbb{N}$ and $\{\varphi_k\}_{k=1}^{\infty}$ be an ONB of $\mathfrak{h}$. We set $F := (F_1, F_2, F_3, F_4)^T$, $G := (G_1, G_2, G_3, G_4)^T$, $f := (f_1, f_2)^T$, and $g := (g_1, g_2)^T$ with $F_i := \sum_{k,l=1}^{M} \mu_{kl}^{(i)} (\varphi_k \otimes \varphi_l)$, $G_i := \sum_{k,l=1}^{M} \nu_{kl}^{(i)} (\varphi_k \otimes \varphi_l) \in \mathfrak{h} \otimes \mathfrak{h}$, $f_j := \sum_{k=1}^{M} \mu_k^{(j)} \varphi_k$, and $g_j := \sum_{k=1}^{M} \nu_k^{(j)} \varphi_k \in \mathfrak{h}$ where the coefficients $\mu_{kl}^{(i)}$, $\nu_{kl}^{(i)}$, $\mu_k^{(j)}$, $\nu_k^{(j)} \in \mathbb{C}$ with $k, l \in \{1, \dots, M\}$, $i \in \{1, 2, 3, 4\}$, $j \in \{1, 2\}$. Then we define the polynomials $\mathcal{P}_1$ and $\mathcal{P}_2$ by

$$\begin{aligned} \mathcal{P}_1(f) &:= \sum_{k=1}^{M} \left(\mu_k^{(1)} a_k^* + \overline{\mu}_k^{(2)} a_k \right), \\ \mathcal{P}_2(F) &:= \sum_{k,l=1}^{M} \left(\mu_{kl}^{(1)} a_k^* a_l^* + \mu_{kl}^{(2)} a_k^* a_l + \mu_{kl}^{(3)} a_k a_l^* + \mu_{kl}^{(4)} a_k a_l \right). \end{aligned} \tag{3.23}$$

Definition 3.29. The generalized two-particle density matrix $\widehat{\Gamma}_\omega$ is defined by

$$\left\langle \begin{pmatrix} G \\ g \\ \mu \end{pmatrix}, \widehat{\Gamma}_\omega \begin{pmatrix} F \\ f \\ \nu \end{pmatrix} \right\rangle_{\mathfrak{H}_{\text{sim}}} := \omega\big((\mathcal{P}_2(F) + \mathcal{P}_1(f) + \nu)\, (\mathcal{P}_2^*(G) + \mathcal{P}_1^*(g) + \overline{\mu}) \big)$$

for any $F, G \in \bigoplus^4 (\mathfrak{h} \otimes \mathfrak{h})$ with $\sum_{k=1}^{\infty} \mu_{kk}^{(3)} < \infty$ and $\sum_{k=1}^{\infty} \nu_{kk}^{(3)} < \infty$, $f, g \in \mathfrak{h} \oplus \mathfrak{h}$, and $\mu, \nu \in \mathbb{C}$ as an operator on $\mathfrak{H}_{\text{sim}}$. The polynomials $\mathcal{P}_1$ and $\mathcal{P}_2$ are of the form specified above in (3.23).

As for the generalized 1-pdm, an easy consequence of the definition are the following properties.

Proposition 3.30. *The generalized two-particle density matrix is selfadjoint and positive semi-definite.*

An explicit form of the generalized 2-pdm as a (7×7)-matrix is given in Appendix A.

2.2 Fermions

The fermion Fock space $\mathcal{F}^- \equiv \mathcal{F}^-[\mathfrak{h}]$ is defined to be the orthogonal sum

$$\mathcal{F}^-[\mathfrak{h}] := \bigoplus_{N=0}^{\infty} \mathfrak{h}^{\wedge N}$$

where for $N \in \mathbb{N}$

$$\mathfrak{h}^{\wedge N} := A_N \mathfrak{h}^{\otimes N}$$

is the antisymmetric tensor product of N copies of $\mathfrak{h}$ and $\mathfrak{h}^{\wedge 0} := \mathbb{C}$. Here the antisymmetrization operator $A \in \mathcal{B}(\mathcal{F})$, $A := \bigoplus_{N=0}^{\infty} A_N$ with $A_N : \mathfrak{h}^{\otimes N} \to \mathfrak{h}^{\otimes N}$ is uniquely defined by

$$A_N (f_1 \otimes \cdots \otimes f_N) := \frac{1}{N!} \sum_{\pi \in \mathfrak{S}_N} (-1)^{\pi} f_1 \otimes \cdots \otimes f_N =: \frac{1}{\sqrt{N!}} f_1 \wedge \cdots \wedge f_N$$

for $f_1, \dots, f_N \in \mathfrak{h}$ where $(-1)^{\pi}$ denotes the sign of the permutation $\pi \in \mathfrak{S}_N$.

Definition 3.31. For any $f \in \mathfrak{h}$ the fermion creation and annihilation operators are denoted by $c^*(f)$ and $c(f)$, respectively. They are bounded operators on $\mathcal{F}^-$. Introducing the anticommutator $\{A, B\} := AB + BA$ they are completely characterized by the properties

$$c(f)\Omega = 0, \quad c^*(f)\Omega = f,$$

and the canonical anticommutation relations (CAR)

$$\begin{aligned}&\{c^*(f), c^*(g)\} = 0, \quad \{c(f), c(g)\} = 0, \quad \text{and}\\ &\{c(f), c^*(g)\} = \langle f, g\rangle_{\mathfrak{h}} \mathbb{1}_{\mathcal{F}^-}\end{aligned}$$

for any $f, g \in \mathfrak{h}$.

Definition 3.32. The C^*-algebra $\mathcal{A}^-$ generated by $\left\{1, c^*(f), c(f) \middle| f \in \mathfrak{h}\right\}$ is called CAR algebra.

Let $\{\varphi_k\}_{k=1}^{\infty}$ be a given ONB of $\mathfrak{h}$ and for this basis $c_k^* \equiv c^*(\varphi_k)$ and $c_k \equiv c(\varphi_k)$. For any $N \in \mathbb{N}$ an ONB of N-particle Hilbert space $\mathfrak{h}^{\wedge N}$ is given by

$$\left\{c_{k_1}^* \cdots c_{k_N}^* \Omega \middle| 1 \leq k_1 < \cdots < k_N\right\}.$$

Moreover,

$$\left\{c_{k_1}^* \cdots c_{k_N}^* \Omega \middle| N \in \mathbb{N} \cup \{0\},\ 1 \leq k_1 < \cdots < k_N\right\}$$

is an ONB of the fermion Fock space $\mathcal{F}^-$. The particle number operator reads

$$\widehat{\mathbb{N}} = \sum_{k=1}^{\infty} c_k^* c_k$$

as a quadratic form for any ONB $\{\varphi_k\}_{k=1}^{\infty}$ of $\mathfrak{h}$.

2.2.1 Fermion Bogoliubov Transformation

In this section we fix an (arbitrary) orthonormal basis $\{\varphi_k\}_{k=1}^{\infty}$ of $\mathfrak{h}$. As the definitions of complex conjugates of both a wave function and an operator depend on the choice of the ONB of $\mathfrak{h}$, so do the transforms defined in the following. We refer the reader to [Sol07] for a basis independent formulation.

Definition 3.33. A linear map $U = \left(\begin{smallmatrix} u & v \\ \overline{v} & \overline{u}\end{smallmatrix}\right) : \mathfrak{h} \oplus \mathfrak{h} \to \mathfrak{h} \oplus \mathfrak{h}$ is called fermion Bogoliubov transformation if $u : \mathfrak{h} \to \mathfrak{h}$ and $v : \mathfrak{h} \to \mathfrak{h}$ are two linear maps fulfilling

$$uu^* + vv^* = \mathbb{1}_{\mathfrak{h}}, \quad u^*u + v^T\overline{v} = \mathbb{1}_{\mathfrak{h}}, \tag{3.24a}$$

$$u^*v + v^T\overline{u} = 0, \quad uv^T + vu^T = 0. \tag{3.24b}$$

Eqs. (3.24a,b) on u and v are equivalent to the condition that U is unitary, i.e.,

$$U^*U = \mathbb{1}_{\mathfrak{h}\oplus\mathfrak{h}}, \quad UU^* = \mathbb{1}_{\mathfrak{h}\oplus\mathfrak{h}}.$$

Therefore the inverse of a fermion Bogoliubov transformation U exists and is the fermion Bogoliubov transformation U^*.

Lemma 3.34. *Let $U = \left(\begin{smallmatrix} u & v \\ \bar{v} & \bar{u} \end{smallmatrix}\right) : \mathfrak{h}\oplus\mathfrak{h} \to \mathfrak{h}\oplus\mathfrak{h}$ be a fermion Bogoliubov transformation. There is a unitary transformation $\mathbb{U}_U : \mathcal{F}^- \to \mathcal{F}^-$ such that*

$$\mathbb{U}_U\left[c^*(f) + c(\overline{g})\right]\mathbb{U}_U^* = c^*(uf + vg) + c(\overline{v\overline{f}} + \overline{u}\overline{g})$$

for all $f \oplus g \in \mathfrak{h}\oplus\mathfrak{h}$ if and only if v is Hilbert–Schmidt.

This condition on v is called Shale-Stinespring condition [SS65]. The proof of this lemma can be found for instance in [Ara71].

2.2.2 States and Density Matrices

Definition 3.35. For fermions, states are continuous linear functionals $\omega \in (\mathcal{A}^-)^*$ on the CAR algebra which are normalized, $\omega(\mathbb{1}_{\mathcal{F}}) = 1$, and positive, $\omega(A) \geq 0$ for all positive semi-definite operators $A \in \mathcal{A}^-$.

Since the fermion systems considered in this work — like atoms and molecules — are particle number-conserving, we only deal with even states, i.e., for every $n \in \mathbb{N}$, we have

$$\omega\big(e(f_1)\cdots e(f_{2n-1})\big) = 0$$

where e denotes either a creation operator c^* or an annihilation operator c. Furthermore we want the particle number expectation value and variance to be finite. Thus, we restrict ourselves to the following subset:

Definition 3.36. We denote the set of all even states with finite particle number variance by

$$\mathcal{Z}^- = \Big\{\omega \in (\mathcal{A}^-)^* \Big|\, \omega \text{ is a state with } \omega\big(\widehat{\mathbb{N}}^2\big) < \infty \\ \text{and } \omega\big(e(f_1)\cdots e(f_{2n-1})\big) = 0 \;\forall\, n \in \mathbb{N}\Big\}.$$

Again e denotes either a creation operator c^* or an annihilation operator c. The subset of all N-particle states is $\mathcal{Z}_N^- := \Big\{\omega \in \mathcal{Z}^- \Big|\, \omega\big(\widehat{\mathbb{N}}\big) = N\Big\}$.

For any state $\omega \in \mathcal{Z}^-$ the particle number expectation value is finite. This can be shown using the Cauchy–Schwarz inequality:

$$\omega\big(\widehat{\mathbb{N}}\big) \leq \sqrt{\omega\big(\widehat{\mathbb{N}}^2\big)} < \infty.$$

Definition 3.37. A state $\omega \in \mathcal{Z}^-$ is called pure if there is a $\Psi \in \mathcal{F}^-$ such that

$$\omega(A) = \langle \Psi, A\Psi\rangle_{\mathcal{F}}$$

for any $A \in \mathcal{A}^-$.

Definition 3.38. A state $\omega \in \mathcal{Z}^-$ is called quasifree, shortly $\omega \in \mathcal{Z}^-_{\mathrm{qf}}$, if it fulfills Wick's Theorem, i.e.,

$$\begin{aligned} &\omega(e_1 e_2 \cdots e_{2n-1}) = 0 \quad \text{and} \\ &\omega(e_1 e_2 \cdots e_{2n}) = \sum_{\pi} (-1)^{\pi} \omega(e_{\pi(1)} e_{\pi(2)}) \cdots \omega(e_{\pi(2n-1)} e_{\pi(2n)}) \end{aligned} \tag{3.25}$$

for every $n \in \mathbb{N}$ where e_i denotes either a creation or an annihilation operator for every $i \in \{1, 2, \ldots, 2n\}$. The sum is taken over all permutations $\pi \in \mathfrak{S}_{2n}$ satisfying

$$\pi(1) < \pi(3) < \cdots < \pi(2n-1) \text{ and } \pi(2k-1) < \pi(2k)$$

for every $k \in \{1, 2, \ldots, n\}$. The right hand side of (3.25) is called Pfaffian.

The subset of the pure quasifree states is denoted by $\mathcal{Z}^-_{\mathrm{pqf}}$. For any $N \in \mathbb{N}$ and any orthonormal vectors $\varphi_1, \ldots, \varphi_N \in \mathfrak{h}$ the vector $\varphi_1 \wedge \cdots \wedge \varphi_N \in \mathcal{F}^-$ is called Slater determinant and defines a pure quasifree state.

The sets $\mathcal{Z}^-_{\mathrm{qf}}$ and $\mathcal{Z}^-_{\mathrm{pqf}}$ are invariant under Bogoliubov transformations.

There is a characterization of pure quasifree states using the Bogoliubov transformation.

Remark 3.39. A state $\omega \in \mathcal{Z}^-$ is pure quasifree if and only if there is a fermion Bogoliubov transformation $U : \mathfrak{h} \oplus \mathfrak{h} \to \mathfrak{h} \oplus \mathfrak{h}$ with unitary representation $\mathbb{U} : \mathcal{F}^- \to \mathcal{F}^-$ such that for any $A \in \mathcal{A}^-$

$$\omega(A) = \langle \mathbb{U}\Omega, A \mathbb{U}\Omega \rangle_{\mathcal{F}} .$$

Since we assume that the fermion states are even, they are in particular centered (see Definition 3.12 for bosons). Moreover for bosons the set of centered quasifree states is a proper subset of the set of quasifree states (Definition 3.13), $\mathcal{Z}^+_{\mathrm{cqf}} \subsetneq \mathcal{Z}^+_{\mathrm{qf}}$, while for fermions all quasifree states are centered.

Definition 3.40. A selfadjoint, positive semi-definite trace class operator $\rho \in \mathcal{L}^1(\mathcal{F}^-)$ of unit trace, $\mathrm{tr}_{\mathcal{F}^-}(\rho) = 1$, is called density matrix.

The map $\mathcal{A}^- \to \mathbb{C}, A \mapsto \mathrm{tr}_{\mathcal{F}^-}(\rho^{\frac{1}{2}} A \rho^{\frac{1}{2}})$ defines a state. Since we only study fermion systems that preserve the particle number, we restrict our attention to density matrices which commute with the particle number operator and have a finite squared particle number expectation value,

$$\rho = \bigoplus_{N=0}^{\infty} \rho^{(N)} \quad \text{and} \quad \mathrm{tr}_{\mathcal{F}^-}(\rho^{\frac{1}{2}} \widehat{\mathbb{N}}^2 \rho^{\frac{1}{2}}) < \infty. \tag{3.26}$$

Note that, if $m, n \geq 0, m \neq n$, then

$$\mathrm{tr}_{\mathcal{F}^-}\left(\rho^{\frac{1}{2}} c^*(f_1) \cdots c^*(f_m)\, c(g_1) \cdots c(g_n)\, \rho^{\frac{1}{2}}\right) = 0$$

for any choice of $f_1, \ldots, f_m, g_1, \ldots, g_n \in \mathfrak{h}$ due to (3.26).

Remark 3.41. In particular for every state $\omega \in \mathcal{Z}^-$ there is a density matrix ρ fulfilling (3.26) and $\mathrm{tr}_{\mathcal{F}^-}(\rho^{\frac{1}{2}} A \rho^{\frac{1}{2}}) = \omega(A)$ for all $A \in \mathcal{A}^-$.

2.2.3 One- and Two-Particle Density Matrices

Based on the fermion states $\omega \in \mathcal{Z}^-$, we can now introduce the notion of fermion one- and two-particle density matrices.

Definition 3.42. For any $\omega \in \mathcal{Z}^-$ the one-particle density matrix (1-pdm) $\gamma_\omega \in \mathcal{B}(\mathfrak{h})$ of ω is defined by

$$\langle f, \gamma_\omega g \rangle_{\mathfrak{h}} := \omega\big(c^*(g)\, c(f)\big)$$

for any $f, g \in \mathfrak{h}$.

Definition 3.43. The two-particle density matrix (2-pdm) $\Gamma_\omega : \mathfrak{h} \otimes \mathfrak{h} \to \mathfrak{h} \otimes \mathfrak{h}$ of a state $\omega \in \mathcal{Z}^-$ is the bounded operator given by

$$\langle f_1 \otimes f_2, \Gamma_\omega\, (g_1 \otimes g_2) \rangle_{\mathfrak{h} \otimes \mathfrak{h}} := \omega\big(c^*(g_2)\, c^*(g_1)\, c(f_1)\, c(f_2)\big)$$

for any $f_1, f_2, g_1, g_2 \in \mathfrak{h}$.

An outline of basic properties of the fermion 1- and 2-pdm can be found in Lemma 2.1 of [BKM12].

2.2.4 Generalized One-Particle Density Matrix for Fermions

Analogously to the boson case we define a generalization of the one-particle density matrix for fermions as in [BLS94]. As for bosons the complex conjugates of a function or of an operator are defined in (3.12) and (3.13), respectively.

Definition 3.44. Let $\omega \in \mathcal{Z}^-$ and fix an ONB $\{\varphi_k\}_{k=1}^\infty$ of $\mathfrak{h}$. Then the generalized one-particle density matrix $\widetilde{\gamma}_\omega$ of ω is an operator on $\mathfrak{h} \oplus \mathfrak{h}$ defined by

$$\langle (f_1 \oplus f_2)\,, \widetilde{\gamma}_\omega\, (g_1 \oplus g_2) \rangle_{\mathfrak{h} \oplus \mathfrak{h}} := \omega\big(\left[c^*(g_1) + c(\overline{g}_2)\right] \left[c(f_1) + c^*(\overline{f}_2)\right]\big)$$

for any $f_1, f_2, g_1, g_2 \in \mathfrak{h}$.

Again we define the operator $\alpha^*_\omega : \mathfrak{h} \to \mathfrak{h}$ for every $f, g \in \mathfrak{h}$ by

$$\langle f, \alpha^*_\omega g \rangle_{\mathfrak{h}} := \omega\big(c^*(g)\, c^*(\overline{f})\big).$$

Then the generalized 1-pdm is expressed as the matrix

$$\widetilde{\gamma}_\omega = \begin{pmatrix} \gamma_\omega & \alpha_\omega \\ \alpha^*_\omega & \mathbb{1}_{\mathfrak{h}} - \overline{\gamma}_\omega \end{pmatrix}.$$

As for bosons the fermion 1-pdm γ is selfadjoint, but α is antisymmetric, i.e., $\alpha^T = -\alpha$, as follows from CAR.

Lemma 3.45. *For any $\omega \in \mathcal{Z}^+$ the generalized one-particle density matrix $\widetilde{\gamma}_\omega$ is a positive semi-definite operator on $\mathfrak{h} \oplus \mathfrak{h}$. In particular it is selfadjoint. Furthermore it is bounded above by $\mathbb{1}_{\mathfrak{h}} \oplus \mathbb{1}_{\mathfrak{h}}$.*

We refer the reader to [BLS94] for a proof. From Lemma 3.45 we deduce $0 \leq \gamma \leq \mathbb{1}_{\mathfrak{h}}$ for the 1-pdm.

A consequence of Wick's Theorem is the following lemma.

Lemma 3.46. *A quasifree state $\omega \in \mathcal{Z}^{-}_{\mathrm{qf}}$ is uniquely determined by its generalized one-particle density matrix $\widetilde{\gamma}_{\omega}$.*

Moreover the generalized 1-pdm transforms in a specific manner under the Bogoliubov transformation.

Lemma 3.47. *Let $\omega \in \mathcal{Z}^{-}$ be a state with generalized one-particle density matrix $\widetilde{\gamma} : \mathfrak{h} \oplus \mathfrak{h} \to \mathfrak{h} \oplus \mathfrak{h}$. For a fermion Bogoliubov transformation $U : \mathfrak{h} \oplus \mathfrak{h} \to \mathfrak{h} \oplus \mathfrak{h}$ with unitary representation $\mathbb{U}_U : \mathcal{F}^{-} \to \mathcal{F}^{-}$ define ω_U by $\omega_U(A) := \omega(\mathbb{U}_U A \mathbb{U}_U^*)$ for any $A \in \mathcal{A}^{-}$. The generalized one-particle density matrix $\widetilde{\gamma}_U$ corresponding to the state ω_U is given by*

$$\widetilde{\gamma}_U = U^* \widetilde{\gamma} U. \tag{3.27}$$

In particular $\widetilde{\gamma}^2 = \widetilde{\gamma}$ implies $\widetilde{\gamma}_U^2 = \widetilde{\gamma}_U$.

Proof. For any $f_1, f_2, g_1, g_2 \in \mathfrak{h}$ we have

$$\begin{aligned}
&\langle (f_1 \oplus f_2), \widetilde{\gamma}_U (g_1 \oplus g_2) \rangle_{\mathfrak{h} \oplus \mathfrak{h}} \\
&\quad = \omega\big(\mathbb{U}_U \left[c^*(g_1) + c(\overline{g}_2)\right] \mathbb{U}_U^* \mathbb{U}_U \left[c(f_1) + c^*(\overline{f}_2)\right] \mathbb{U}_U^*\big) \\
&\quad = \omega\big(\left[c^*(ug_1 + vg_2) + c(u\overline{g}_2 + v\overline{g}_1)\right] \left[c(uf_1 + vf_2) + c^*(u\overline{f}_2 + v\overline{f}_1)\right]\big) \\
&\quad = \langle U (g_1 \oplus g_2), \widetilde{\gamma}\, U (f_1 \oplus f_2) \rangle_{\mathfrak{h} \oplus \mathfrak{h}}
\end{aligned}$$

for the matrix elements of $\widetilde{\gamma}_U$. Thus (3.27) holds. Furthermore by the unitarity of U and (3.27) we obtain $\widetilde{\gamma}_U^2 = U^* \widetilde{\gamma} U U^* \widetilde{\gamma} U = U^* \widetilde{\gamma}^2 U$ and $\widetilde{\gamma}^2 = \widetilde{\gamma}$ yields $\widetilde{\gamma}_U^2 = U^* \widetilde{\gamma} U = \widetilde{\gamma}_U$. □

2.3 Bogoliubov–Hartree–Fock Theory

2.3.1 Boson Bogoliubov–Hartree–Fock Theory

For bosons the number of particles in most physically relevant models is not fixed. As, for instance, in a system of photons interacting with an electron, photons can appear or disappear depending on what is energetically favorable. The particle number should therefore not be fixed in the variational process yielding the ground state energy $E_{\mathrm{gs}} := \inf\{\sigma(\mathbb{H})\}$. By the Rayleigh–Ritz principle the ground state energy (as well as the ground state) is determined by

$$E_{\mathrm{gs}} = \inf\left\{\omega(\mathbb{H}) \,\middle|\, \omega \in \mathcal{Z}^{+}\right\}.$$

In Bogoliubov–Hartree–Fock (BHF) theory, also called generalized Hartree–Fock theory, the variation is restricted to quasifree states:

$$E_{\mathrm{BHF}} := \inf\left\{\omega(\mathbb{H}) \,\middle|\, \omega \in \mathcal{Z}^{+}_{\mathrm{qf}}\right\}.$$

The BHF energy E_{BHF} is an upper bound to the ground state energy E_{gs}. Note that, unlike the common definitions of quasifreeness, our quasifree states are not necessarily centered. Since a quasifree state is uniquely determined by its further generalized 1-pdm $\widehat{\gamma}_\omega$, there is a functional $\mathcal{E}_{\mathrm{BHF}} : \mathcal{D}(\mathcal{E}_{\mathrm{BHF}}) \to \mathbb{C}$, $\mathcal{D}(\mathcal{E}_{\mathrm{BHF}}) \subseteq \mathcal{B}(\mathfrak{h} \oplus \mathfrak{h} \oplus \mathbb{C})$, called Bogoliubov–Hartree–Fock energy functional, such that $\mathcal{E}_{\mathrm{BHF}}(\widehat{\gamma}_\omega) = \omega(\mathbb{H})$. Thus the BHF energy is rewritten as

$$E_{\mathrm{BHF}} = \inf\left\{\mathcal{E}_{\mathrm{BHF}}(\widehat{\gamma}_\omega)\middle|\, \omega \in \mathcal{Z}_{\mathrm{qf}}^+\right\} = \inf\left\{\mathcal{E}_{\mathrm{BHF}}(\widehat{\gamma})\middle|\, \widehat{\gamma} \geq 0,\ \mathrm{tr}_{\mathfrak{h}}(\gamma) < \infty\right\}.$$

The second equality is a consequence of two facts: On the one hand, any quasifree state ω with first moment b is linked to a unique centered quasifree state via the Weyl transformation $\mathbb{W}_b$. On the other hand, any positive semi-definite operator $\widetilde{\gamma} = \begin{pmatrix} \gamma & \alpha \\ \alpha^* & \mathbb{1}_{\mathfrak{h}}+\overline{\gamma} \end{pmatrix}$ on $\mathfrak{h} \oplus \mathfrak{h}$ fulfilling $\mathrm{tr}(\gamma) < \infty$ is the generalized 1-pdm of a centered quasifree state, cf. [Nam11].

2.3.2 Fermion Bogoliubov–Hartree–Fock Theory

For fermions assume $U : \mathbb{R}^3 \to \mathbb{R}$ to be an external potential and $V : \mathbb{R}^3 \times \mathbb{R}^3 \to \mathbb{R}_0^+$ a repulsive interaction between two particles. There are multiplication operators associated to these potentials which we also denote by U and V, respectively. With the Laplace operator Δ the Hamiltonian of the system is given by

$$H^{(N)} := \sum_{i=1}^{N} \left[-\Delta_i - U(x_i)\right] + \sum_{1 \leq i < j \leq N} V(x_i, x_j),$$

where $x_i \in \mathbb{R}^3$, $1 \leq i \leq N$. We only allow for potentials for which $H^{(N)}$ is defined as a selfadjoint operator on a dense domain $\mathcal{D}_N$ and is bounded below. Examples of a system represented by such a Hamiltonian are atoms and molecule. The second quantization of this Hamiltonian is

$$\mathbb{H} = \sum_{i,j=1}^{\infty} h_{ij} c_i^* c_j + \frac{1}{2} \sum_{i,j,k,l=1}^{\infty} V_{ij,kl} c_j^* c_i^* c_k c_l$$

where the one-particle operator h and the interaction operator V are given by

$$h_{ij} := \langle \varphi_i, (-\Delta - U)\, \varphi_j \rangle_{\mathfrak{h}},$$
$$V_{ij,kl} := \langle \varphi_i \otimes \varphi_j, V\,(\varphi_k \otimes \varphi_l) \rangle_{\mathfrak{h}\otimes\mathfrak{h}},$$

respectively, for any elements of a given ONB $\{\varphi_i\}_{i=1}^{\infty}$ of $\mathfrak{h}$ with $\|\nabla \varphi_i\|_{\mathfrak{h}} < \infty$. The Hamiltonian $H^{(N)}$ is the restriction of $\mathbb{H}$ to the N-particle Fock space $\mathfrak{h}^{\wedge N}$. If we do not assume the dynamics to conserve the particle number, the ground state energy of the N-particle system is determined by the Rayleigh–Ritz principle:

$$E_{\mathrm{gs}} = \inf\left\{\omega(\mathbb{H})\middle|\, \omega \in \mathcal{Z}^-\right\}.$$

Using the energy functional

$$\mathcal{E}(\gamma, \Gamma) := \mathrm{tr}_{\mathfrak{h}}(h\gamma) + \frac{1}{2}\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}(V\Gamma),$$

this can be re-expressed as

$$E_{\mathrm{gs}} = \inf\left\{\mathcal{E}(\gamma,\Gamma)\,\middle|\,(\gamma,\Gamma) \text{ is representable}\right\}.$$

Here the problem of representability arises, i.e., a classification of all representable operator pairs on $\mathfrak{h} \times (\mathfrak{h}\otimes\mathfrak{h})$. In order to obtain an upper bound to E_{gs}, the variation is restricted to quasifree states which yields the Bogoliubov–Hartree–Fock energy

$$\begin{aligned} E_{\mathrm{BHF}} &:= \inf\left\{\omega(\mathbb{H})\,\middle|\,\omega \in \mathcal{Z}^{-}_{\mathrm{qf}}\right\} \\ &= \inf\left\{\mathcal{E}_{\mathrm{BHF}}(\widetilde{\gamma})\,\middle|\,\mathbb{1}_{\mathfrak{h}\oplus\mathfrak{h}} \geq \widetilde{\gamma} \geq 0,\ \mathrm{tr}_{\mathfrak{h}}(\gamma) < \infty\right\}. \end{aligned}$$

For any quasifree state ω the Bogoliubov–Hartree–Fock functional $\mathcal{E}_{\mathrm{BHF}}$ is given by $\mathcal{E}_{\mathrm{BHF}}(\widetilde{\gamma}_\omega) := \omega(\mathbb{H})$ where $\widetilde{\gamma}_\omega$ is the generalized 1-pdm of ω.

3 Bosonic Representability Conditions and the Generalized Two-Particle Density Matrix

3.1 Particle Number-Conserving Systems

To our knowledge sets of representability conditions given in the literature are for particle number-conserving systems for fermions, as well as for bosons. I.e. only states that fulfill

$$\omega\left(\left[\prod_{k=1}^{n} a^*(f_k)\right]\left[\prod_{l=1}^{m} a(g_l)\right]\right) = 0$$

for any two sets $\{f_k\}_{k=1}^n, \{g_l\}_{l=1}^m \subseteq \mathfrak{h}$ with $m, n \in \mathbb{N}\cup\{0\}$ and $m \neq n$ are considered.

Since the dynamics of many realistic physical boson systems do not conserve the particle number, an alternative should be found. We first restate some representability conditions for bosons.

Definition 3.48. Let (γ, Γ) be a pair of operators on $\mathfrak{h}$ and $\mathfrak{h}\otimes\mathfrak{h}$, respectively. We say that (γ,Γ) satisfies the representability conditions up to second order with particle number-conservation if

1. (γ,Γ) is admissible,
2. Γ satisfies the P-condition, i.e.,

$$\Gamma \geq 0,$$

and

3. the G-condition, i.e., for any $A \in \mathcal{B}(\mathfrak{h})$ we have

$$\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left((A^* \otimes A) [\Gamma + \mathrm{Ex}\,(\gamma \otimes \mathbb{1}_{\mathfrak{h}})] \right) \geq |\mathrm{tr}_{\mathfrak{h}}\,(A\gamma)|^2.$$

These conditions can be found, e.g., in [GP64, GM04]. Note that these conditions are only necessary conditions, but do not ensure that the considered operators are one- and two-particle density matrices. Furthermore, we omit here other known conditions like the T_1- and T_2-condition, cf. [Erd78b].

Remark 3.49. The Q-condition is omitted since it follows from the P-condition and the positivity of γ, see [GM04]. Nevertheless we can similarly rephrase the Q-condition from [GM04] as

$$\Gamma \geq -\left(\mathbb{1}_{\mathfrak{h}\otimes\mathfrak{h}} + \mathrm{Ex}\right)\left(\gamma \otimes \mathbb{1}_{\mathfrak{h}} + \mathbb{1}_{\mathfrak{h}} \otimes \gamma + \mathbb{1}_{\mathfrak{h}} \otimes \mathbb{1}_{\mathfrak{h}}\right).$$

The representability conditions for bosons up to second order can be derived in the same spirit as it is done for fermions in Section 3 of Chapter 4 (see also [BKM12]).

Theorem 3.50. *Let ω be a linear continuous functional on $\mathcal{A}^+$ with $\omega(\mathbb{1}_{\mathcal{F}}) = 1$, $\omega(\widehat{\mathbb{N}}^2) < \infty$, and $\omega(e_1 \ldots e_{2N-1}) = 0$ for all $N \in \mathbb{N}$, where e_k denotes either a creation or annihilation operator. Furthermore, let Γ_ω and γ_ω be the corresponding one- and two-particle density matrices and $\{\varphi_k\}_{k=1}^\infty$ an ONB of $\mathfrak{h}$. Then the following statements are equivalent:*

(i) For any polynomial $\mathcal{P}_r \in \mathcal{A}^+$ in creation and annihilation operators of degree $r \leq 2$ we have

$$\omega(\mathcal{P}_r \mathcal{P}_r^*) \geq 0.$$

(ii) $\gamma_\omega \geq 0$ and Γ_ω fulfills the G- and P-condition.

Since the proof is analogous to the fermion case considered in [BKM12], we omit the details here. Note that, unlike the fermion case, the trace class conditions on the 1- and 2-pdm cannot be derived from the polynomials since the boson creation and annihilation operators are unbounded.

3.2 Systems without Particle Number-Conservation and the Generalized Two-Particle Density Matrix

We generalize the definition of the representability conditions up to second order to systems — and, thus, states — which do not conserve the particle number. These representability conditions arise in the same manner as those for particle conserving states by considering expectation values of polynomials up to second order in the creation and annihilation operators. Due to the absence of particle number-conservation the expectation values of terms, in which the number of creation operators is not equal to the number of annihilation operators, do in general not vanish. A simple consequence of Definition 3.29 is the following proposition.

Proposition 3.51. *The representability conditions up to second order are satisfied if the pair* (γ, Γ) *of operators on* $\mathfrak{h}$ *and* $\mathfrak{h} \otimes \mathfrak{h}$*, respectively, is admissible and* $\widehat{\Gamma}$ *is positive semi-definite as an operator on* $\mathfrak{H}_{\rm sim}$*.*

Let ω be a linear functional on the operators on $\mathcal{F}^+$. Since, on the one hand, any polynomial up to second order in creation and annihilation operators can be written as $\mathcal{P} = \mathcal{P}_2(F) + \mathcal{P}_1(f) + \nu$ with $F \in \bigoplus^4 \mathfrak{h}^{\otimes 2}$, $f \in \bigoplus^2 \mathfrak{h}$, $\nu \in \mathbb{C}$, Definition 3.29 yields

$$\omega(\mathcal{P}\mathcal{P}^*) = \left\langle \begin{pmatrix} F \\ f \\ \nu \end{pmatrix}, \widehat{\Gamma} \begin{pmatrix} F \\ f \\ \nu \end{pmatrix} \right\rangle .$$

On the other hand, every element of $\mathfrak{H}_{\rm sim}$ can be written as a vector with $F \in \bigoplus^4 \mathfrak{h}^{\otimes 2}$, $f \in \bigoplus^2 \mathfrak{h}$, $\nu \in \mathbb{C}$. Thus, the representability conditions up to second order are exactly those arising from

$$\omega(\mathcal{P}\mathcal{P}^*) \geq 0$$

for any polynomial $\mathcal{P}$ in creation and annihilation operators of degree $r \leq 2$.

In Appendix B we show that a polynomial of degree two in boson creation and annihilation operators can be simplified using a Bogoliubov–Weyl transformation if the coefficients satisfy certain conditions. Unfortunately, these conditions are quite restrictive such that the lemma proven in Appendix B does not yield a simplification of Proposition 3.51.

Remark 3.52. Since the generalized 1-pdm appears as a block in the generalized 2-pdm, it inherits the definiteness property from the generalized 2-pdm.

If one varies only over particle number-conserving states, then $\widehat{\Gamma}$ assumes a block-diagonal form and the complexity of the representability reduces considerably. In fact only three independent conditions remain which are reminiscent of the G- and P-condition in quantum chemistry (see Theorem 3.50).

4 Variation over Pure Quasifree States and the Bogoliubov–Hartree–Fock Energy

For bosons Theorem I.2 of [BBT13] states for the Pauli–Fierz model that the Bogoliubov–Hartree–Fock energy coincides with the infimum of the energy functional for a variation over pure quasifree states. We prove a more general statement which holds for bosons, as well as for fermions. The main result of this section is the following

Theorem 3.53. *Assume the Hamiltonian* $\mathbb{H}$ *to be bounded below. Then*

$$E_{\rm BHF} = \inf \left\{ \omega(\mathbb{H}) \,\middle|\, \omega \text{ is pure and quasifree} \right\} =: E_{\rm BHF}^{\rm pure}.$$

We show the statement in the following two subsections for bosons and fermions separately.

4.1 Bosons

A more precise statement of Theorem 3.53 for bosons is:

Theorem 3.54. *Let $\mathbb{H}$ be a Hamiltonian on $\mathcal{F}^+$ that is bounded below. Then*

$$E_{\text{BHF}} = \inf\left\{ \omega(\mathbb{H}) \middle| \omega \in \mathcal{Z}^+_{\text{pqf}} \right\} =: E^{\text{pure}}_{\text{BHF}}.$$

In order to prove the theorem, we need some properties of quasifree and pure quasifree states. To this end we give a characterization of quasifree and pure quasifree states using the Bogoliubov transformation.

Lemma 3.55. *For any quasifree density matrix there are a positive semi-definite operator $C \in \mathcal{L}^1(\mathfrak{h})$ with $\|C\|_{\mathcal{B}(\mathfrak{h})} < 1$ and second quantization $\Gamma(C) := \bigoplus_{N=0}^\infty C^{\otimes N}$, a boson Bogoliubov transformation with unitary implementation $\mathbb{U}$, and $f \in \mathfrak{h}$ such that*

$$\rho = \mathbb{W}_f \mathbb{U} \frac{\Gamma(C)}{\text{tr}_{\mathcal{F}^+}(\Gamma(C))} \mathbb{U}^* \mathbb{W}_f^*.$$

If in addition the density matrix is pure, it is of the form $\mathbb{W}_f \mathbb{U} |\Omega\rangle \langle\Omega| \mathbb{U}^* \mathbb{W}_f^*$ where we used the Dirac bra-ket notation.

This Lemma is a consequence of Lemma III.1 in [BBT13].

Proof (Proof of Theorem 3.54). Without loss of generality we assume the Hamiltonian to be positive semi-definite. If $\mathbb{H}$ is bounded below, there is a constant $\mu \geq 0$ such that $\mathbb{H}_0 := \mathbb{H} + \mu \mathbb{1}_{\mathcal{F}^+} \geq 0$. Considering $\mathbb{H}_0$ instead of $\mathbb{H}$ just adds the constant μ to both E_{BHF} and $E^{\text{pure}}_{\text{BHF}}$.

The inequality

$$E_{\text{BHF}} = \inf\left\{ \omega(\mathbb{H}) \middle| \omega \in \mathcal{Z}^+_{\text{qf}} \right\} \leq \inf\left\{ \omega(\mathbb{H}) \middle| \omega \in \mathcal{Z}^+_{\text{pqf}} \right\} = E^{\text{pure}}_{\text{BHF}}$$

follows from the definition of the BHF energy since the variation is restricted to the proper subset $\mathcal{Z}^+_{\text{pqf}} \subsetneq \mathcal{Z}^+_{\text{qf}}$.

It remains to prove that $\omega(\mathbb{H}) \geq E^{\text{pure}}_{\text{BHF}}$ for any quasifree state $\omega \in \mathcal{Z}^+_{\text{qf}}$. Let $\omega \in \mathcal{Z}^+_{\text{qf}}$ with $\omega(\mathbb{H}) < \infty$ and denote the corresponding density matrix by ρ. Then

$$\omega(\mathbb{H}) = \text{tr}_{\mathcal{F}^+}\left(\rho^{\frac{1}{2}} \mathbb{H} \rho^{\frac{1}{2}}\right) = \text{tr}_{\mathcal{F}^+}\left(\left(\rho^{\frac{1}{2}} \mathbb{H}^{\frac{1}{2}}\right) \left(\mathbb{H}^{\frac{1}{2}} \rho^{\frac{1}{2}}\right) \right)$$

since $\mathbb{H} \geq 0$. Therefore $\rho^{\frac{1}{2}} \mathbb{H}^{\frac{1}{2}}$ is Hilbert–Schmidt and we obtain by the cyclicity of the trace

$$\text{tr}_{\mathcal{F}^+}\left(\left(\rho^{\frac{1}{2}} \mathbb{H}^{\frac{1}{2}}\right) \left(\mathbb{H}^{\frac{1}{2}} \rho^{\frac{1}{2}}\right) \right) = \text{tr}_{\mathcal{F}^+}\left(\mathbb{H}^{\frac{1}{2}} \rho \mathbb{H}^{\frac{1}{2}}\right).$$

Since $\mathbb{H}$ is selfadjoint, there is an ONB $\{\Psi_k\}_{k=1}^\infty$ of $\mathcal{F}^+$ such that $\Psi_k \in \mathcal{D}(\mathbb{H})$ for any $k \in \mathbb{N}$. Then

$$\text{tr}_{\mathcal{F}^+}\left(\mathbb{H}^{\frac{1}{2}} \rho \mathbb{H}^{\frac{1}{2}}\right) = \sum_{k=1}^\infty \left\langle \mathbb{H}^{\frac{1}{2}} \Psi_k, \rho \mathbb{H}^{\frac{1}{2}} \Psi_k \right\rangle_{\mathcal{F}}.$$

By Lemma 3.55 the positive semi-definite operator ρ can be written as $\rho = \kappa\kappa^*$ where

$$\kappa := \mathbb{W}_f \mathbb{U} \frac{\Gamma(C^{\frac{1}{2}})}{[\mathrm{tr}_{\mathcal{F}^+}(\Gamma(C))]^{\frac{1}{2}}}$$

with some $f \in \mathfrak{h}$, a Bogoliubov transformation with unitary implementation $\mathbb{U}$, and some $C \in \mathcal{L}^1(\mathfrak{h}), C \geq 0, \|C\|_{\mathcal{B}(\mathfrak{h})} < 1$. Hence,

$$\omega(\mathbb{H}) = \sum_{k=1}^{\infty} \left\| \kappa^* \mathbb{H}^{\frac{1}{2}} \Psi_k \right\|_{\mathcal{F}}^2. \tag{3.28}$$

We continue by introducing a resolution of the identity with coherent states. To this end we consider an increasing sequence of n-dimensional Hilbert spaces $\mathfrak{h}_n \subseteq \mathfrak{h}_{n+1} \subseteq \mathfrak{h}$, $n \in \mathbb{N}$, with $\overline{\bigcup_{n\in\mathbb{N}} \mathfrak{h}_n} = \mathfrak{h}$ and $C\mathfrak{h}_n \subseteq \mathfrak{h}_n$. For any n-dimensional Hilbert space $\mathfrak{h}_n$ there is an isometric isomorphism $I : \mathfrak{h}_n \to \mathbb{C}^n$. We define the measure $\mathrm{d}\mu_n(z^{(n)})$ on $\mathfrak{h}_n$ by $\int_{\mathfrak{h}_n} \mathrm{d}\mu_n(z^{(n)}) f(z^{(n)}) := \int_{\mathbb{C}^n} \frac{\mathrm{d}^n x \mathrm{d}^n y}{\pi^n} f(Iz^{(n)})$ where $x := \mathrm{Re}(z)$, $y := \mathrm{Im}(z)$. For any $n \in \mathbb{N}$ we have $\mathfrak{h} = \mathfrak{h}_n \oplus \mathfrak{h}_n^\perp$ where $\mathfrak{h}_n^\perp$ denotes the orthogonal complement of $\mathfrak{h}_n$ in $\mathfrak{h}$. Moreover $\mathcal{F}^+ \cong \mathcal{F}^+[\mathfrak{h}_n] \otimes \mathcal{F}^+[\mathfrak{h}_n^\perp]$ and $\Omega = \Omega_n \otimes \Omega_n^\perp$ with $\Omega_n \in \mathcal{F}^+[\mathfrak{h}_n]$ and $\Omega_n^\perp \in \mathcal{F}^+[\mathfrak{h}_n^\perp]$. For every $n \in \mathbb{N}$ the projections $\left|\mathbb{W}(z^{(n)})\Omega\right\rangle \left\langle \mathbb{W}(z^{(n)})\Omega\right|$, $z^{(n)} \in \mathfrak{h}_n$, satisfy

$$\mathbb{1}_{\mathcal{F}^+[\mathfrak{h}_n]} \otimes \left|\Omega_n^\perp\right\rangle \left\langle \Omega_n^\perp\right| = \int_{\mathfrak{h}_n} \mathrm{d}\mu_n(z^{(n)}) \left|\mathbb{W}(z^{(n)})\Omega\right\rangle \left\langle \mathbb{W}(z^{(n)})\Omega\right|,$$

see, e.g., [Ber66, CR12]. Consequently

$$\langle \Psi, \Psi \rangle_{\mathcal{F}} = \lim_{n\to\infty} \int_{\mathfrak{h}_n} \mathrm{d}\mu_n(z^{(n)}) |\left\langle \Psi, \mathbb{W}(z^{(n)})\Omega \right\rangle_{\mathcal{F}}|^2$$

for any $\Psi \in \mathcal{F}^+$. Thus each summand of the right hand side of (3.28) is rewritten as

$$\left\| \kappa^* \mathbb{H}^{\frac{1}{2}} \Psi_k \right\|_{\mathcal{F}}^2 = \lim_{n\to\infty} \int_{\mathfrak{h}_n} \mathrm{d}\mu_n(z^{(n)}) |\left\langle \mathbb{H}^{\frac{1}{2}} \Psi_k, \kappa \mathbb{W}(z^{(n)})\Omega \right\rangle_{\mathcal{F}}|^2.$$

The sequence $\left(k \mapsto \int_{\mathfrak{h}_n} \mathrm{d}\mu_n(z^{(n)}) |\left\langle \mathbb{H}^{\frac{1}{2}} \Psi_k, \kappa \mathbb{W}(z^{(n)})\Omega \right\rangle_{\mathcal{F}}|^2\right)_{n=1}^{\infty}$ is monotonously increasing. Therefore the summation and the limit can be exchanged by the monotone convergence theorem where the summation is considered as an integral with the counting measure. Thus we get

$$\omega(\mathbb{H}) = \lim_{n\to\infty} \sum_{k=1}^{\infty} \int_{\mathfrak{h}_n} \mathrm{d}\mu_n(z^{(n)}) |\left\langle \mathbb{H}^{\frac{1}{2}} \Psi_k, \kappa \mathbb{W}(z^{(n)})\Omega \right\rangle_{\mathcal{F}}|^2.$$

Afterwards Fubini's Theorem yields

$$\begin{aligned}\omega(\mathbb{H}) &= \lim_{n\to\infty} \int_{\mathfrak{h}_n} \mathrm{d}\mu_n(z^{(n)}) \sum_{k=1}^{\infty} |\left\langle \mathbb{H}^{\frac{1}{2}} \Psi_k, \kappa \mathbb{W}(z^{(n)})\Omega \right\rangle_{\mathcal{F}}|^2 \\ &= \lim_{n\to\infty} \int_{\mathfrak{h}_n} \mathrm{d}\mu_n(z^{(n)}) \left\langle \kappa \mathbb{W}(z^{(n)})\Omega, \mathbb{H}\kappa \mathbb{W}(z^{(n)})\Omega \right\rangle_{\mathcal{F}}\end{aligned}$$

and we conclude from the proof of Lemma III.7 in [BBT13] that

$$\kappa \mathbb{W}(z^{(n)})\Omega = \mathbb{W}_f \mathbb{U} \frac{\Gamma(C^{\frac{1}{2}})}{[\mathrm{tr}_{\mathcal{F}^+}(\Gamma(C))]^{\frac{1}{2}}} \mathbb{W}(z^{(n)})\Omega = \nu_C(z^{(n)}) \mathbb{W}_g \mathbb{U}\Omega$$

for some $g \in \mathfrak{h}$ and $\nu_C(z^{(n)}) \in \mathbb{C}$ with $\lim_{n\to\infty} \int_{\mathfrak{h}_n} \mathrm{d}\mu_n(z^{(n)}) |\nu_C(z^{(n)})|^2 = 1$. By Lemma 3.55 this vector defines a pure quasifree state and consequently

$$\begin{aligned}
\omega(\mathbb{H}) &= \lim_{n\to\infty} \int_{\mathfrak{h}_n} \mathrm{d}\mu_n(z^{(n)}) \left\langle \kappa \mathbb{W}(z^{(n)})\Omega, \mathbb{H}\kappa \mathbb{W}(z^{(n)})\Omega \right\rangle_{\mathcal{F}} \\
&\geq E_{\mathrm{BHF}}^{\mathrm{pure}} \lim_{n\to\infty} \int_{\mathfrak{h}_n} \mathrm{d}\mu_n(z^{(n)}) |\nu_C\left(z^{(n)}\right)|^2 \\
&= E_{\mathrm{BHF}}^{\mathrm{pure}}
\end{aligned}$$

which completes the proof. □

4.2 Fermions

For fermions a similar result to Theorem 3.54 holds:

Theorem 3.56. *Let $\mathbb{H}$ be a Hamiltonian on $\mathcal{F}^-$ that is bounded below. Then*

$$E_{\mathrm{BHF}} = \inf\left\{\omega(\mathbb{H}) \middle| \omega \in \mathcal{Z}_{\mathrm{pqf}}^-\right\} =: E_{\mathrm{BHF}}^{\mathrm{pure}}.$$

Before we prove this theorem, we need two preparatory lemmas.

Lemma 3.57. *Let $\omega \in \mathcal{Z}_{\mathrm{qf}}^-$ with density matrix ρ. Then there are a decomposition $\mathfrak{h} = \mathfrak{h}_S \oplus^{\perp} \mathfrak{h}_\Gamma$ with $n := \dim(\mathfrak{h}_S) < \infty$, a positive semi-definite trace class operator $B \in \mathcal{B}(\mathfrak{h}_\Gamma)$, and a fermion Bogoliubov transformation U with unitary implementation $\mathbb{U}$ such that*

$$\rho = \mathbb{U}_U \left((|\varphi_1 \wedge \cdots \wedge \varphi_n\rangle \langle \varphi_1 \wedge \cdots \wedge \varphi_n|) \otimes \frac{\Gamma(B)}{\mathrm{tr}_{\mathcal{F}^-}(\Gamma(B))} \right) \mathbb{U}_U^* \tag{3.29}$$

for any ONB $\{\varphi_k\}_{k=1}^n$ of $\mathfrak{h}_S$.

Proof. It is known that there are fermion Bogoliubov transformations U such that the generalized 1-pdm of $\rho_U := \mathbb{U}_U^* \rho \mathbb{U}_U$ is of the form

$$\widetilde{\gamma}_U = \begin{pmatrix} \gamma_U & 0 \\ 0 & \mathbb{1}_{\mathfrak{h}} - \overline{\gamma}_U \end{pmatrix} \tag{3.30}$$

for some $0 \leq \gamma_U \leq \mathbb{1}_{\mathfrak{h}}$ with $\mathrm{tr}_{\mathfrak{h}}(\gamma_U) < \infty$, see, e.g., [BLS94, Theorem 2.3]. Let $\mathfrak{h}_S$ be the eigenspace of γ_U associated to the eigenvalue 1 with dimension $n < \infty$ and $\mathfrak{h}_\Gamma$ its orthogonal complement. Then $\gamma_U = P_S + \gamma_\Gamma$ where P_S is the orthogonal projection on $\mathfrak{h}_S$ and γ_Γ the restriction of γ_U to $\mathfrak{h}_\Gamma$. Note that γ_Γ satisfies $\mathfrak{h}_S \subseteq \ker(\gamma_\Gamma)$, $\gamma_\Gamma \mathfrak{h}_\Gamma \subseteq \mathfrak{h}_\Gamma$, and $0 \leq \gamma_\Gamma \leq \mu \mathbb{1}_{\mathfrak{h}}$ for some $0 < \mu < 1$. Let $\varphi_1, \ldots, \varphi_n$ be an ONB of $\mathfrak{h}_S$. Moreover let

$$\rho' := |\varphi_1 \wedge \cdots \wedge \varphi_n\rangle \langle \varphi_1 \wedge \cdots \wedge \varphi_n| \otimes \frac{\Gamma(B)}{\mathrm{tr}_{\mathcal{F}^-}(\Gamma(B))}$$

with $B := (\gamma_\Gamma)\left(\mathbb{1}_{\mathfrak{h}_\Gamma} - \gamma_\Gamma\right)^{-1}$. In order to show that $\rho' = \rho_U$, it is sufficient to observe that ρ' defines a quasifree state ω' and $\widetilde{\gamma}_{\omega'} = \widetilde{\gamma}_U$ from (3.30) since quasifree states are characterized by their generalized 1-pdm, see [BLS94]. Note that we implicitly used the decomposition $\mathcal{F}^- \cong \mathcal{F}^-[\mathfrak{h}_S] \otimes \mathcal{F}^-[\mathfrak{h}_\Gamma]$. □

Remark 3.58. For any positive semi-definite operator $B \in \mathcal{L}^1(\mathfrak{h}_\Gamma)$ there are an ONB $\{\phi_k\}_{k=1}^\infty$ of $\mathfrak{h}_\Gamma$ and coefficients $b_k \geq 0$, $k \in \mathbb{N}$ such that $B = \sum_{k=1}^\infty b_k |\phi_k\rangle\langle\phi_k|$ and $\sum_{k=1}^\infty b_k < \infty$. Thus

$$\mathrm{tr}_{\mathcal{F}^-}\left(\Gamma(B)\right) = \mathrm{tr}_{\mathcal{F}^-}\left(\bigotimes_{k=1}^\infty \Gamma(b_k)\right) = \prod_{k=1}^\infty \mathrm{tr}_{\mathcal{F}^-}\left(\Gamma(b_k)\right) = \prod_{k=1}^\infty (1 + b_k)$$

which converges due to $\sum_{k=1}^\infty b_k < \infty$. Here $\Gamma(b_k)$ should be understood as the second quantized operator $\Gamma(b_k |\phi_k\rangle\langle\phi_k|)$ on $\mathcal{F}^-[\mathbb{C}\phi_k]$.

Lemma 3.59. *Let $\omega \in \mathcal{Z}_{\mathrm{qf}}^-$ with density matrix ρ. Then there is a sequence $(\rho_k)_{k=1}^\infty$ of pure quasifree density matrices and a sequence $(\lambda_k)_{k=1}^\infty \in [0,\infty)^{\mathbb{N}}$ with $\sum_{k=1}^\infty \lambda_k < \infty$ such that*

$$\langle \Psi_1, \rho \Psi_2\rangle_{\mathcal{F}} = \lim_{n\to\infty} \left\langle \Psi_1, \sum_{k=1}^n \lambda_k \rho_k \Psi_2 \right\rangle_{\mathcal{F}}$$

for any $\Psi_1, \Psi_2 \in \mathcal{F}^-$. I.e., every quasifree state is a convex combination of pure quasifree states.

Proof. From Lemma 3.57 we know that every quasifree density matrix is of the form (3.29) and we use the notation specified there in the following. We complete $\{\varphi_k\}_{k=1}^n$ to an ONB $\{\varphi_k\}_{k=1}^\infty$ of $\mathfrak{h}$ where $\{\varphi_k\}_{k=n+1}^\infty$ is an ONB of $\mathfrak{h}_\Gamma$. Then

$$\langle \Psi, \Phi\rangle_{\mathcal{F}} = \lim_{N\to\infty} \lim_{M\to\infty} \sum_{k=0}^N \sum_{1\leq i_1 < \cdots < i_k \leq M} \langle \Psi, \varphi_{i_1} \wedge \cdots \wedge \varphi_{i_k}\rangle_{\mathcal{F}} \times \langle \varphi_{i_1} \wedge \cdots \wedge \varphi_{i_k}, \Phi\rangle_{\mathcal{F}} \tag{3.31}$$

for any $\Psi, \Phi \in \mathcal{F}^-$. Choosing the ONB $\{\varphi_k\}_{k=n+1}^\infty$ of $\mathfrak{h}_\Gamma$ such that B is diagonalized and using (3.31), we obtain in the weak sense

$$\begin{aligned}\kappa^2 &:= \left(|\varphi_1 \wedge \cdots \wedge \varphi_n\rangle\langle\varphi_1 \wedge \cdots \wedge \varphi_n| \otimes \frac{\Gamma(B^{\frac12})}{[\mathrm{tr}_{\mathcal{F}^-}(\Gamma(B))]^{\frac12}} \right)^2 \\ &= \lim_{M,N\to\infty} \sum_{k=n+1}^N \sum_{n+1\leq i_1<\cdots<i_k\leq M} (|\varphi_1 \wedge \cdots \wedge \varphi_n\rangle\langle\varphi_1 \wedge \cdots \wedge \varphi_n|) \\ &\quad \otimes \left(\frac{\Gamma(B^{\frac12})}{[\mathrm{tr}_{\mathcal{F}^-}(\Gamma(B))]^{\frac12}} |\varphi_{i_1} \wedge \cdots \wedge \varphi_{i_k}\rangle\langle\varphi_{i_1} \wedge \cdots \wedge \varphi_{i_k}| \frac{\Gamma(B^{\frac12})}{[\mathrm{tr}_{\mathcal{F}^-}(\Gamma(B))]^{\frac12}} \right).\end{aligned}$$

This can be written as

$$\kappa^2 = \frac{1}{\mathrm{tr}_{\mathcal{F}^-}(\Gamma(B))} \lim_{M,N\to\infty} \sum_{k=n+1}^{N} \sum_{n+1\le i_1<\cdots<i_k\le M} (|\varphi_1 \wedge \cdots \wedge \varphi_n\rangle$$
$$\langle \varphi_1 \wedge \cdots \wedge \varphi_n|) \otimes \left|B^{\frac{1}{2}}\varphi_{i_1} \wedge \cdots \wedge B^{\frac{1}{2}}\varphi_{i_k}\right\rangle \left\langle B^{\frac{1}{2}}\varphi_{i_1} \wedge \cdots \wedge B^{\frac{1}{2}}\varphi_{i_k}\right|$$
$$= \frac{1}{\mathrm{tr}_{\mathcal{F}^-}(\Gamma(B))} \lim_{M,N\to\infty} \sum_{k=n+1}^{N} \sum_{n+1\le i_1<\cdots<i_k\le M}$$
$$\left|\varphi_1 \wedge \cdots \wedge \varphi_n \wedge B^{\frac{1}{2}}\varphi_{i_1} \wedge \cdots \wedge B^{\frac{1}{2}}\varphi_{i_k}\right\rangle$$
$$\times \left\langle \varphi_1 \wedge \cdots \wedge \varphi_n \wedge B^{\frac{1}{2}}\varphi_{i_1} \wedge \cdots \wedge B^{\frac{1}{2}}\varphi_{i_k}\right|.$$

Each operator

$$\left|\varphi_1 \wedge \cdots \wedge \varphi_n \wedge B^{\frac{1}{2}}\varphi_{i_1} \wedge \cdots \wedge B^{\frac{1}{2}}\varphi_{i_k}\right\rangle$$
$$\times \left\langle \varphi_1 \wedge \cdots \wedge \varphi_n \wedge B^{\frac{1}{2}}\varphi_{i_1} \wedge \cdots \wedge B^{\frac{1}{2}}\varphi_{i_k}\right|$$

is either equal to zero or a pure quasifree density matrix (up to a normalization constant). Finally a pure quasifree density matrix conjugated by a Bogoliubov transformation is a pure quasifree state, too, which completes the proof. □

Now we are prepared to prove Theorem 3.56. Since the proof is to a large extend similar to the proof of Theorem 3.54, we only give details where there are differences.

Proof (Proof of Theorem 3.56). Again without loss of generality we assume that the Hamiltonian is positive semi-definite.

As for bosons the inequality

$$E_{\mathrm{BHF}} = \inf\left\{\omega(\mathbb{H})\,\middle|\,\omega \in \mathcal{Z}_{\mathrm{qf}}^-\right\} \le \inf\left\{\omega(\mathbb{H})\,\middle|\,\omega \in \mathcal{Z}_{\mathrm{pqf}}^-\right\} = E_{\mathrm{BHF}}^{\mathrm{pure}}$$

is immediate.

Thus we show $\omega(\mathbb{H}) \ge E_{\mathrm{BHF}}^{\mathrm{pure}}$ for any $\omega \in \mathcal{Z}_{\mathrm{qf}}^-$. Let $\omega \in \mathcal{Z}_{\mathrm{qf}}^-$ with $\omega(\mathbb{H}) < \infty$ and denote the corresponding density matrix by ρ. Furthermore let $\{\Psi_k\}_{k=1}^{\infty}$ be an ONB of $\mathcal{F}^-$ such that $\Psi_k \in \mathcal{D}(\mathbb{H})$ for any $k \in \mathbb{N}$. Analogously to the boson case we obtain

$$\mathrm{tr}_{\mathcal{F}^-}\left(\mathbb{H}^{\frac{1}{2}}\rho\mathbb{H}^{\frac{1}{2}}\right) = \sum_{k=1}^{\infty} \left\langle \mathbb{H}^{\frac{1}{2}}\Psi_k, \rho\mathbb{H}^{\frac{1}{2}}\Psi_k\right\rangle_{\mathcal{F}}.$$

By Lemma 3.57 the positive semi-definite operator ρ can be written as $\rho = \kappa\kappa^*$ where

$$\kappa := \mathbb{U}_U\left[|\varphi_1 \wedge \cdots \wedge \varphi_n\rangle\langle\varphi_1 \wedge \cdots \wedge \varphi_n| \otimes \frac{\Gamma(B^{\frac{1}{2}})}{[\mathrm{tr}_{\mathcal{F}^-}(\Gamma(B))]^{\frac{1}{2}}}\right]$$

with a decomposition $\mathfrak{h} = \mathfrak{h}_S \oplus^{\perp} \mathfrak{h}_\Gamma$, $n := \dim(\mathfrak{h}_S) < \infty$, an ONB $\{\varphi_k\}_{k=1}^n$ of $\mathfrak{h}_S$, a unitarily implementable Bogoliubov transformation U, and a positive semi-definite trace class operator $B \in \mathcal{B}(\mathfrak{h}_\Gamma)$. Hence

$$\omega(\mathbb{H}) = \sum_{k=1}^{\infty} \left\| \kappa^* \mathbb{H}^{\frac{1}{2}} \Psi_k \right\|_{\mathcal{F}}^2 .$$

Instead of a resolution of the identity by coherent states for bosons we use the resolution of the identity by Slater determinants,

$$\mathbb{1}_{\mathcal{F}^-} = \lim_{N\to\infty} \lim_{M\to\infty} \sum_{l=0}^{N} \sum_{1\le i_1<\cdots<i_l\le M} \left| \varphi_{i_1} \wedge \cdots \wedge \varphi_{i_l} \right\rangle \left\langle \varphi_{i_1} \wedge \cdots \wedge \varphi_{i_l} \right| ,$$

as in the proof of Lemma 3.59, in particular, Eq. (3.31). Then we obtain

$$\omega(\mathbb{H}) = \sum_{k=1}^{\infty} \lim_{N\to\infty} \lim_{M\to\infty} \sum_{l=0}^{N} \sum_{1\le i_1<\cdots<i_l\le M} \left| \left\langle \mathbb{H}^{\frac{1}{2}} \Psi_k, \kappa\left(\varphi_{i_1} \wedge \cdots \wedge \varphi_{i_l}\right) \right\rangle_{\mathcal{F}} \right|^2 .$$

Because the sequence

$$\left(k \mapsto \lim_{M\to\infty} \sum_{l=0}^{N} \sum_{1\le i_1<\cdots<i_l\le M} \left| \left\langle \mathbb{H}^{\frac{1}{2}} \Psi_k, \kappa\left(\varphi_{i_1} \wedge \cdots \wedge \varphi_{i_l}\right) \right\rangle_{\mathcal{F}} \right|^2 \right)_{N=1}^{\infty}$$

is monotonously increasing, the monotone convergence theorem allows for an exchange of the k-summation and the first limit. Using the monotone convergence theorem a second time to exchange the second limit and the k-summation, we obtain

$$\omega(\mathbb{H}) = \lim_{N\to\infty} \lim_{M\to\infty} \sum_{k=1}^{\infty} \sum_{l=0}^{N} \sum_{1\le i_1<\cdots<i_l\le M} \left| \left\langle \mathbb{H}^{\frac{1}{2}} \Psi_k, \kappa\left(\varphi_{i_1} \wedge \cdots \wedge \varphi_{i_l}\right) \right\rangle_{\mathcal{F}} \right|^2 .$$

Furthermore we can change the order of the summations since the sum is absolutely convergent and get

$$\begin{aligned} &\omega(\mathbb{H}) \\ &= \lim_{N\to\infty} \lim_{M\to\infty} \sum_{l=0}^{N} \sum_{1\le i_1<\cdots<i_l\le M} \left\langle \kappa\left(\varphi_{i_1} \wedge \cdots \wedge \varphi_{i_l}\right), \mathbb{H}\kappa\left(\varphi_{i_1} \wedge \cdots \wedge \varphi_{i_l}\right) \right\rangle_{\mathcal{F}} . \end{aligned}$$

Every vector $\kappa\left(\varphi_{i_1} \wedge \cdots \wedge \varphi_{i_l}\right)$ defines a pure quasifree state, cf. the proof of Lemma 3.59. Since

$$\langle \Psi, \mathbb{H}\Psi \rangle_{\mathcal{F}} \ge E_{\mathrm{BHF}}^{\mathrm{pure}}$$

for any pure quasifree state $\Psi \in \mathcal{F}^-$, we finally have

$$\begin{aligned} \omega(\mathbb{H}) &\ge E_{\mathrm{BHF}}^{\mathrm{pure}} \lim_{M,N\to\infty} \sum_{l=0}^{N} \sum_{1\le i_1<\cdots<i_l\le M} \left\langle \varphi_{i_1} \wedge \cdots \wedge \varphi_{i_l}, \rho\left(\varphi_{i_1} \wedge \cdots \wedge \varphi_{i_l}\right) \right\rangle_{\mathcal{F}} \\ &= E_{\mathrm{BHF}}^{\mathrm{pure}} . \end{aligned}$$

This proves the assertion. □

Theorem 3.53 now follows from the Theorems 3.54 and 3.56.

5 Pure Quasifree States and their Generalized One-Particle Density Matrix

For a given generalized fermion 1-pdm $\widetilde{\gamma}$ it is known that there is a pure quasifree state ω which has $\widetilde{\gamma}$ as its generalized 1-pdm if and only if the generalized 1-pdm is a projection, i.e., $\widetilde{\gamma}^2 = \widetilde{\gamma}$ (see Section 5.2). For bosons a similar statement is also known. In this section we show that an even stronger relation holds:

Theorem 3.60. *The following statements are equivalent:*

(i) ω *is a centered pure quasifree state.*

(ii) *The generalized one-particle density matrix* $\widetilde{\gamma}$ *corresponding to* ω *satisfies* $\mathrm{tr}_{\mathfrak{h}}(\gamma) < \infty$ *and*

$$\widetilde{\gamma}\mathcal{S}\widetilde{\gamma} = -\widetilde{\gamma} \quad \text{for bosons,}$$
$$\widetilde{\gamma}^2 = \widetilde{\gamma} \quad \text{for fermions.}$$

Recall $\mathcal{S} = \mathbb{1}_{\mathfrak{h}} \oplus (-\mathbb{1}_{\mathfrak{h}}) \in \mathcal{B}(\mathfrak{h} \oplus \mathfrak{h})$. A proof of Theorem 3.60 in the boson case is given in the following subsection. Two consequences of this theorem are discussed afterwards. In the second subsection we prove the statement for fermions.

5.1 Bosons

Before we show Theorem 3.60 for bosons, we give some preparatory lemmas.

Lemma 3.61. *If an operator* $\widetilde{\gamma} = \begin{pmatrix} \gamma & \alpha \\ \alpha^* & \mathbb{1}_{\mathfrak{h}}+\overline{\gamma} \end{pmatrix} : \mathfrak{h} \oplus \mathfrak{h} \to \mathfrak{h} \oplus \mathfrak{h}$ *satisfies* $\widetilde{\gamma} \geq 0$, $\mathrm{tr}_{\mathfrak{h}}(\gamma) < \infty$, *and*

$$\widetilde{\gamma}\mathcal{S}\widetilde{\gamma} = -\widetilde{\gamma}, \tag{3.32}$$

there is a centered pure quasifree state $\omega \in \mathcal{Z}^+_{\mathrm{pqf}} \cap \mathcal{Z}^+_{\mathrm{cen}}$ *that has* $\widetilde{\gamma}$ *as its generalized one-particle density matrix. Furthermore let* $\omega \in \mathcal{Z}^+_{\mathrm{pqf}} \cap \mathcal{Z}^+_{\mathrm{cen}}$ *be a centered pure quasifree state. Then the corresponding generalized one-particle density matrix* $\widetilde{\gamma}$ *fulfills* (3.32).

For a proof see, e.g., [Nam11, Sol07]. Equation (3.32) is rewritten in a single equation for operators on $\mathfrak{h}$, i.e., we do not need the matrices $\widetilde{\gamma}$ and $\mathcal{S}$.

Proposition 3.62. *Let* $\omega \in \mathcal{Z}^+$ *be a state with the generalized one-particle density matrix* $\widetilde{\gamma} = \begin{pmatrix} \gamma & \alpha \\ \alpha^* & \mathbb{1}_{\mathfrak{h}}+\overline{\gamma} \end{pmatrix}$. *Then the following statements are equivalent:*

(i) $\widetilde{\gamma}\mathcal{S}\widetilde{\gamma} = -\widetilde{\gamma}$.

(ii) $\gamma^2 + \gamma = \alpha\alpha^*$.

Proof. Computing and simplifying the matrix products of (i), we obtain the four equations

$$\gamma^2 + \gamma = \alpha\alpha^*, \tag{3.33}$$
$$\overline{\gamma}^2 + \overline{\gamma} = \alpha^*\alpha, \tag{3.34}$$
$$\gamma\alpha = \alpha\overline{\gamma}, \tag{3.35}$$
$$\alpha^*\gamma = \overline{\gamma}\alpha^*. \tag{3.36}$$

Thus the implication $(i) \Rightarrow (ii)$ is immediate. It remains to prove $(ii) \Rightarrow (i)$. Equation (3.36) is the adjoint of (3.35), and (3.34) is equivalent to (3.33). The system of equations therefore reduces to (3.33) and (3.35). Furthermore we show that (3.35) follows from (3.33). We define $f : \mathbb{R}^+ \to \mathbb{R}^+$ by $f(y) := \sqrt{y + 1/4} - 1/2$ and observe that f is the inverse map of $x \mapsto x + x^2$, $\mathbb{R}^+ \to \mathbb{R}^+$. Then

$$\gamma = f(\alpha\alpha^*) \text{ and } \overline{\gamma} = f(\overline{\alpha\alpha^*}) = f(\alpha^*\alpha).$$

Since $\alpha\alpha^*$ is bounded, we approximate the function f by a sequence of polynomials $(p_n)_{n=1}^{\infty}$, i.e., $\lim_{n\to\infty} p_n(x) = f(x)$ uniformly on the compact interval $\left[-\|\alpha\alpha^*\|_{\text{op}}, \|\alpha\alpha^*\|_{\text{op}}\right] \subsetneq \mathbb{R}$. So $p_n(\alpha\alpha^*)$ and $p_n(\alpha^*\alpha)$ are well-defined. Using $(\alpha\alpha^*)^m \alpha = \alpha (\alpha^*\alpha)^m$ for all $m \in \mathbb{N}$ and limits in operator norm, we obtain

$$\gamma\alpha = f(\alpha\alpha^*)\alpha = \lim_{n\to\infty} p_n(\alpha\alpha^*)\alpha = \lim_{n\to\infty} \alpha p_n(\alpha^*\alpha) = \alpha f(\alpha^*\alpha) = \alpha\overline{\gamma}$$

which proves the assertion. □

Remark 3.63. In [BBT13]

$$\gamma = \frac{1}{2}\left(\cosh(2r) - \mathbb{1}_{\mathfrak{h}}\right), \quad \hat{\alpha} = \frac{1}{2}\sinh(2r)$$

are used where $\langle f, \hat{\alpha}\overline{g}\rangle_{\mathfrak{h}} = \langle f, \alpha g\rangle_{\mathfrak{h}}$ and $r : \mathfrak{h} \to \mathfrak{h}$ is an antilinear operator. r obeys $\langle f, rg\rangle_{\mathfrak{h}} = \langle g, rf\rangle_{\mathfrak{h}}$ for any $f, g \in \mathfrak{h}$ and r^2 is trace class. These two equations are, however, implied by (3.33) and in turn yield (3.35).

Centered pure quasifree states can be characterized by a Bogoliubov transformation (see [Nam11] for the proof):

Lemma 3.64. *A centered boson state $\omega \in \mathcal{Z}^+_{\text{cen}}$ is pure quasifree if and only if there is a boson Bogoliubov transformation $U : \mathfrak{h} \oplus \mathfrak{h} \to \mathfrak{h} \oplus \mathfrak{h}$ with unitary representation $\mathbb{U}_U : \mathcal{F}^+ \to \mathcal{F}^+$ such that for any $A \in \mathcal{A}^+$*

$$\omega(A) = \langle \mathbb{U}_U\Omega, A\mathbb{U}_U\Omega\rangle_{\mathcal{F}}.$$

The relation between a generalized 1-pdm fulfilling (3.32) and the corresponding centered pure quasifree state is even closer.

Lemma 3.65. *Let $\omega \in \mathcal{Z}^+_{\text{cen}}$ and assume that the corresponding generalized one-particle density matrix $\widetilde{\gamma}$ satisfies*

$$\widetilde{\gamma}\mathcal{S}\widetilde{\gamma} = -\widetilde{\gamma}. \tag{3.37}$$

Then ω is a centered pure quasifree state.

Proof. As stated in Remark 3.22, the generalized 1-pdm is of the form $\widetilde{\gamma} = \begin{pmatrix} \gamma & \alpha \\ \alpha^* & \mathbb{1}_{\mathfrak{h}} + \overline{\gamma} \end{pmatrix}$ where $\gamma : \mathfrak{h} \to \mathfrak{h}$ is the 1-pdm and $\alpha^* : \mathfrak{h} \to \mathfrak{h}$ is defined in (3.18). For any $k \in \mathbb{N}$ let ϕ_k denote an eigenfunction corresponding to the eigenvalue λ_k of γ, i.e., $\gamma\phi_k = \lambda_k\phi_k$. Since the 1-pdm is selfadjoint, we choose a set of eigenfunctions $\{\phi_k\}_{k=1}^{\infty}$ which forms an ONB of $\mathfrak{h}$. We define the operators $u : \mathfrak{h} \to \mathfrak{h}$ and $v : \mathfrak{h} \to \mathfrak{h}$ by

$$u\phi_k := (\mathbb{1} + \gamma)^{\frac{1}{2}} \phi_k := (1 + \lambda_k)^{\frac{1}{2}} \phi_k \quad \text{and}$$
$$v\phi_k := \alpha (\mathbb{1} + \overline{\gamma})^{-\frac{1}{2}} \phi_k := (1 + \lambda_k)^{-\frac{1}{2}} \alpha\phi_k$$

where we abbreviate $\mathbb{1} \equiv \mathbb{1}_{\mathfrak{h}}$ in this proof. We show that

$$U := \begin{pmatrix} u & v \\ \overline{v} & \overline{u} \end{pmatrix} = \begin{pmatrix} (\mathbb{1} + \gamma)^{\frac{1}{2}} & \alpha (\mathbb{1} + \overline{\gamma})^{-\frac{1}{2}} \\ \alpha^* (\mathbb{1} + \gamma)^{-\frac{1}{2}} & (\mathbb{1} + \overline{\gamma})^{\frac{1}{2}} \end{pmatrix}$$

defines a boson Bogoliubov transformation. To this end we prove the conditions on u and v specified in Definition 3.5. We know from the proof of Proposition 3.62 that (3.37) is equivalent to (3.33)–(3.36). Using $\alpha\overline{\gamma} = \gamma\alpha$ and $\alpha\alpha^* = \gamma + \gamma^2$, we calculate

$$uu^* - vv^* = \mathbb{1} + \gamma - (\mathbb{1} + \gamma)^{-1} \alpha\alpha^* = \mathbb{1}$$

which is the left equation of (3.14a). The right equation of (3.14a) is derived from

$$u^*u - v^T\overline{v} = (\mathbb{1} + \gamma)^{\frac{1}{2}} (\mathbb{1} + \gamma)^{\frac{1}{2}} - (\mathbb{1} + \gamma)^{-\frac{1}{2}} \alpha^T\overline{\alpha} (\mathbb{1} + \gamma)^{-\frac{1}{2}}$$

and using $\alpha^T = \alpha$ and $\alpha\alpha^* = \gamma^2 + \gamma$. Furthermore,

$$u^*v - v^T\overline{u} = (\mathbb{1} + \gamma)^{\frac{1}{2}} \alpha (\mathbb{1} + \overline{\gamma})^{-\frac{1}{2}} - (\mathbb{1} + \gamma)^{-\frac{1}{2}} \alpha (\mathbb{1} + \overline{\gamma})^{\frac{1}{2}} = 0$$

because $\alpha^T = \alpha$ and $\alpha\overline{\gamma} = \gamma\alpha$. Thus we get the left equation of (3.14b). Analogously we obtain

$$uv^T - vu^T = (\mathbb{1} + \gamma)^{\frac{1}{2}} (\mathbb{1} + \gamma)^{-\frac{1}{2}} \alpha^T - \alpha (\mathbb{1} + \overline{\gamma})^{-\frac{1}{2}} (\mathbb{1} + \overline{\gamma})^{\frac{1}{2}} = 0.$$

Hence, U is a boson Bogoliubov transformation. Since

$$\begin{aligned} \mathrm{tr}_{\mathfrak{h}}(v^*v) &= \mathrm{tr}_{\mathfrak{h}}\big((\mathbb{1} + \overline{\gamma})^{-\frac{1}{2}} \alpha^*\alpha (\mathbb{1} + \overline{\gamma})^{-\frac{1}{2}} \big) = \mathrm{tr}_{\mathfrak{h}}(\overline{\gamma}) \\ &= \mathrm{tr}_{\mathfrak{h}}(\gamma) = \omega(\widehat{\mathbb{N}}) < \infty, \end{aligned}$$

there is a unitary implementation $\mathbb{U} : \mathcal{F}^+ \to \mathcal{F}^+$ of the Bogoliubov transformation U by Lemma 3.7.

We define a state $\omega_U \in \mathcal{Z}^+$ by $\omega_U(A) := \omega(\mathbb{U}A\mathbb{U}^*)$ for any $A \in \mathcal{A}^+$. We show that the generalized 1-pdm of ω_U is

$$\widetilde{\gamma}_U = \begin{pmatrix} 0 & 0 \\ 0 & \mathbb{1} \end{pmatrix}. \tag{3.38}$$

Since $\widetilde{\gamma}_U = U^* \widetilde{\gamma} U$ by Lemma 3.24, (3.38) is equivalent to

$$\begin{pmatrix} \gamma & \alpha \\ \alpha^* & \mathbb{1} + \overline{\gamma} \end{pmatrix} = U \begin{pmatrix} 0 & 0 \\ 0 & \mathbb{1} \end{pmatrix} U^* = \begin{pmatrix} vv^* & vu^T \\ \overline{u}v^* & \overline{u}u^T \end{pmatrix}.$$

Thus we only verify that $\gamma = vv^*$ and $\alpha = vu^T$. On the one hand,

$$vv^* = \alpha \left(\mathbb{1} + \overline{\gamma}\right)^{-1} \alpha^* = \left(\mathbb{1} + \gamma\right)^{-1} \alpha\alpha^* = \gamma$$

with $\alpha\overline{\gamma} = \gamma\alpha$ and $\alpha\alpha^* = \gamma + \gamma^2$. On the other hand,

$$vu^T = \alpha \left(\mathbb{1} + \overline{\gamma}\right)^{-\frac{1}{2}} \left(\mathbb{1} + \overline{\gamma}\right)^{\frac{1}{2}} = \alpha.$$

Therefore the Bogoliubov transformation U yields $\widetilde{\gamma}_U = \left(\begin{smallmatrix} 0 & 0 \\ 0 & \mathbb{1} \end{smallmatrix}\right)$. In particular we have

$$\gamma_U = 0 \tag{3.39}$$

and $\widetilde{\gamma}_U \mathcal{S} \widetilde{\gamma}_U = -\widetilde{\gamma}_U$.

Next we show that the only state having $\widetilde{\gamma}_U$ as its generalized 1-pdm is the vacuum state. We choose $\{\varphi_n\}_{n=1}^{\infty}$ to be a fixed, but arbitrary ONB of $\mathfrak{h}$. We consider the set

$$\mathcal{K} := \left\{ K : \mathbb{N} \to \mathbb{N} \cup \{0\} \,\middle|\, \exists n_0 \in \mathbb{N} \text{ s.t. } \forall n \geq n_0 : \ K_n = 0 \right\}$$

and define for any $K \in \mathcal{K}$

$$a_K^* := \prod_{\substack{n=1 \\ K_n \neq 0}}^{\infty} \frac{\left(a_n^*\right)^{K_n}}{\sqrt{K_n!}}$$

and $\Psi_K \in \mathcal{F}^+$ by $\Psi_K := a_K^* \Omega$. Note that $\Psi_{(0,0,\dots)} = \Omega$. For any $K, L \in \mathcal{K}$ with $K \neq L$ we have $\langle \Psi_K, \Psi_L \rangle = 0$ and $\langle \Psi_K, \Psi_K \rangle = 1$, and $\{\Psi_K\}_{K \in \mathcal{K}} \subset \mathcal{F}^+$ forms an ONB of the boson Fock space, the so-called occupancy number basis.

We denote by ρ_U the density matrix corresponding to ω_U. With the occupancy number representation and the usual Dirac bra-ket notation we rewrite the density matrix ρ_U of the state ω_U as

$$\rho_U = \sum_{K,L \in \mathcal{K}} \mu_{K,L} \left|\Psi_K\right\rangle \left\langle \Psi_L\right|$$

where $\mu_{K,L} := \omega_U(|\Psi_L\rangle \langle \Psi_K|) \in \mathbb{C}$. For any $n \in \mathbb{N}$ and any $K \in \mathcal{K}$ with $K_n \geq 1$ we denote the vector, in which one of the particles in the state given by φ_n is removed, by $K - E^{(n)}$ where $E^{(n)} \in \mathcal{K}$ with $E_n^{(n)} = 1$ and $E_m^{(n)} = 0$ for all $m \in \mathbb{N}$, $m \neq n$. Then for all $n \in \mathbb{N}$ and $K, L \in \mathcal{K}$ with $K_n \geq 1$ the Cauchy–Schwarz inequality yields

$$\begin{aligned} |\mu_{K,L}|^2 &= |\omega_U\big(|\Psi_L\rangle \left\langle \Psi_{K-E^{(n)}} \right| \frac{1}{\sqrt{K_n}} a_n \big)|^2 \\ &\leq \frac{1}{K_n} \omega_U\big(|\Psi_L\rangle \left\langle \Psi_{K-E^{(n)}}, \Psi_{K-E^{(n)}} \right\rangle_{\mathcal{F}} \langle \Psi_L| \big) \omega_U(a_n^* a_n) \end{aligned}$$

which vanishes since by (3.39) $\omega_U(a_n^* a_n) = \langle \varphi_n, \gamma_U \varphi_n \rangle_{\mathfrak{h}} = 0$ for all $n \in \mathbb{N}$. Consequently $\mu_{K,L} = 0$ if any $K, L \in \mathcal{K}$ is different from $(0, 0, \dots)$, and $\mu_{K,K} = 1$ for $K = (0, 0, \dots)$. As asserted we have

$$\omega_U(A) = \langle \Omega, A\Omega \rangle_{\mathcal{F}}$$

for any $A \in \mathcal{A}^+$. Hence we obtain

$$\omega(A) = \omega_U(\mathbb{U}^* A \mathbb{U}) = \langle \mathbb{U}\Omega, A\mathbb{U}\Omega \rangle_{\mathcal{F}}$$

for the original state ω. So ω has to be a centered pure quasifree state according to Lemma 3.64. ☐

Let $\widetilde{\gamma}$ be a generalized 1-pdm fulfilling (3.37) and $U : \mathfrak{h} \oplus \mathfrak{h} \to \mathfrak{h} \oplus \mathfrak{h}$ a boson Bogoliubov transformation with unitary implementation $\mathbb{U} : \mathcal{F}^+ \to \mathcal{F}^+$ that yields

$$\widetilde{\gamma}_U = U^* \widetilde{\gamma} U = \begin{pmatrix} \gamma_U & 0 \\ 0 & \mathbb{1} + \overline{\gamma}_U \end{pmatrix}.$$

By the second assertion of Lemma 3.24 (3.37) implies

$$\widetilde{\gamma}_U \mathcal{S} \widetilde{\gamma}_U = -\widetilde{\gamma}_U.$$

So γ_U satisfies

$$\begin{pmatrix} \gamma_U^2 & 0 \\ 0 & -\mathbb{1} - 2\overline{\gamma}_U - \overline{\gamma}_U^2 \end{pmatrix} = \begin{pmatrix} -\gamma_U & 0 \\ 0 & -\mathbb{1} - \overline{\gamma}_U \end{pmatrix}$$

or equivalently $\gamma_U^2 = -\gamma_U$. Since γ_U is positive semi-definite, we conclude

$$\gamma_U = 0$$

and $\widetilde{\gamma}_U$ is of the form (3.38).

We conclude from Lemmas 3.61 and 3.65:

Theorem 3.66. *Let $\omega \in \mathcal{Z}^+_{\text{cen}}$ be a centered state and $\mathcal{S} = \mathbb{1}_{\mathfrak{h}} \oplus (-\mathbb{1}_{\mathfrak{h}}) \in \mathcal{B}(\mathfrak{h} \oplus \mathfrak{h})$. Then the following statements are equivalent:*

(i) *ω is a pure quasifree state.*

(ii) *The generalized one-particle density matrix $\widetilde{\gamma}$ of $\omega \in \mathcal{Z}^+$ fulfills $\mathrm{tr}_{\mathfrak{h}}(\gamma) < \infty$ and*

$$\widetilde{\gamma} \mathcal{S} \widetilde{\gamma} = -\widetilde{\gamma}.$$

Proof. The implication $(i) \Rightarrow (ii)$ is given by the second assertion of Lemma 3.61 and the reverse by Lemma 3.65. ☐

A consequence of Lemma 3.65 is the following corollary.

Corollary 3.67. *Let $\omega \in \mathcal{Z}^+$ be a state and*

$$\widehat{\gamma} = \begin{pmatrix} \gamma & \alpha & b \\ \alpha^* & \mathbb{1}_\mathfrak{h} + \overline{\gamma} & \overline{b} \\ b^* & \overline{b}^* & 1 \end{pmatrix}$$

the corresponding further generalized 1-pdm with $\gamma : \mathfrak{h} \to \mathfrak{h}$ and $\alpha^* : \mathfrak{h} \to \mathfrak{h}$ as defined in Eqs. (3.16) and (3.18), respectively. As in (3.22) the first moment $b \in \mathfrak{h}$ of the state ω is given by $\langle f, b \rangle_\mathfrak{h} := \omega\big(a(f)\big)$ for any $f \in \mathfrak{h}$. Furthermore, we define the selfadjoint operator $\mathcal{Q}_f : \mathfrak{h} \oplus \mathfrak{h} \oplus \mathbb{C} \to \mathfrak{h} \oplus \mathfrak{h} \oplus \mathbb{C}$ by

$$\mathcal{Q}_f := \begin{pmatrix} \mathbb{1}_\mathfrak{h} & 0 & -f \\ 0 & -\mathbb{1}_\mathfrak{h} & \overline{f} \\ -f^* & \overline{f}^* & -1 \end{pmatrix}$$

for any $f \in \mathfrak{h}$. If

$$\widehat{\gamma} \mathcal{Q}_b \widehat{\gamma} = -\widehat{\gamma}, \tag{3.40}$$

then ω is a pure quasifree state.

Proof. If ω is centered, we have $b = 0$ and (3.40) reduces to $\widehat{\gamma}\mathcal{Q}_0\widehat{\gamma} = -\widehat{\gamma}$ which is equivalent to (3.37). So Lemma 3.65 directly yields the assertion. Now we do not assume the state to be centered. Then for the Weyl transformation $\mathbb{W}_b : \mathcal{F}^+ \to \mathcal{F}^+$ we define the state $\omega_0 \in \mathcal{Z}^+$ by $\omega_0(A) := \omega\big(\mathbb{W}_b^* A\, \mathbb{W}_b\big)$ for any $A \in \mathcal{A}^+$. First we show that $b_0 = 0$, $\gamma_0 = \gamma - |b\rangle\langle b|$, and $\alpha_0^* = \alpha^* - |\overline{b}\rangle\langle b|$ for this state ω_0. For any $f \in \mathfrak{h}$ we have

$$\langle b_0, f \rangle_\mathfrak{h} := \omega_0\big(a^*(f)\big) = \omega\big(a^*(f) - \langle b, f\rangle_\mathfrak{h} \mathbb{1}_{\mathcal{F}^+}\big) = \langle b, f \rangle_\mathfrak{h} - \langle b, f \rangle_\mathfrak{h} = 0.$$

Thus $b_0 = 0$ and ω_0 is a centered state. Furthermore, for any $f, g \in \mathfrak{h}$

$$\begin{aligned} \langle f, \gamma_0 g \rangle_\mathfrak{h} &:= \omega_0\big(a^*(g)\, a(f)\big) \\ &= \omega\big(\big[a^*(g) - \langle b, g \rangle_\mathfrak{h} \mathbb{1}_{\mathcal{F}^+}\big]\big[a(f) - \langle f, b \rangle_\mathfrak{h} \mathbb{1}_{\mathcal{F}^+}\big]\big) \\ &= \langle f, \gamma g \rangle_\mathfrak{h} - \langle f, b \rangle_\mathfrak{h} \langle b, g \rangle_\mathfrak{h} . \end{aligned}$$

An analogous calculation yields

$$\begin{aligned} \left\langle \overline{f}, \alpha_0^* g \right\rangle_\mathfrak{h} &:= \omega_0\big(a^*(g)\, a^*(f)\big) \\ &= \omega\big(\big[a^*(g) - \langle b, g \rangle_\mathfrak{h} \mathbb{1}_{\mathcal{F}^+}\big]\big[a^*(f) - \langle b, f \rangle_\mathfrak{h} \mathbb{1}_{\mathcal{F}^+}\big]\big) \\ &= \omega\big(a^*(g)\, a^*(f)\big) - \langle b, g \rangle_\mathfrak{h} \langle b, f \rangle_\mathfrak{h} . \end{aligned}$$

Next we consider (3.40). For every $f \in \mathfrak{h}$ we decompose the operator $\mathcal{Q}_f$ as

$$\mathcal{Q}_f = \mathcal{R}_f \widehat{\mathcal{S}} \mathcal{R}_f^*$$

where the operators $\mathcal{R}_f, \widehat{\mathcal{S}} : \mathfrak{h} \oplus \mathfrak{h} \oplus \mathbb{C} \to \mathfrak{h} \oplus \mathfrak{h} \oplus \mathbb{C}$ are given by

$$\mathcal{R}_f := \begin{pmatrix} -\mathbb{1}_\mathfrak{h} & 0 & 0 \\ 0 & -\mathbb{1}_\mathfrak{h} & 0 \\ f^* & \overline{f}^* & 1 \end{pmatrix} \quad \text{and} \quad \widehat{\mathcal{S}} := \begin{pmatrix} \mathbb{1}_\mathfrak{h} & 0 & 0 \\ 0 & -\mathbb{1}_\mathfrak{h} & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

Since $\mathcal{R}_b$ is invertible, (3.40) is equivalent to

$$\left(\mathcal{R}_b^*\widehat{\gamma}\mathcal{R}_b\right)\widehat{\mathcal{S}}\left(\mathcal{R}_b^*\widehat{\gamma}\mathcal{R}_b\right) = -\mathcal{R}_b^*\widehat{\gamma}\mathcal{R}_b. \tag{3.40'}$$

A straightforward computation yields

$$\mathcal{R}_b^*\widehat{\gamma}\mathcal{R}_b = \begin{pmatrix} \gamma - |b\rangle\langle b| & \alpha - |b\rangle < big|\overline{b}| & 0 \\ \alpha^* - |\overline{b}\rangle\langle b| & \mathbb{1}_{\mathfrak{h}} + \overline{\gamma} - \left|\overline{b}\right\rangle\left\langle\overline{b}\right| & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Summarizing the results, we obtain

$$\mathcal{R}_b^*\widehat{\gamma}\mathcal{R}_b = \begin{pmatrix} \gamma_0 & \alpha_0 & 0 \\ \alpha_0^* & \mathbb{1}_{\mathfrak{h}} + \overline{\gamma}_0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

which is the further generalized 1-pdm $\widehat{\gamma}_0$ of the state ω_0. Thus (3.40) implies

$$\widehat{\gamma}_0\widehat{\mathcal{S}}\widehat{\gamma}_0 = -\widehat{\gamma}_0.$$

Since the upper left 2×2-matrix of $\widehat{\gamma}_0$ (which is an operator on $\mathfrak{h}\oplus\mathfrak{h}$) is the generalized 1-pdm $\widetilde{\gamma}_0$ and $\widehat{\mathcal{S}}$ is diagonal, we find

$$\widetilde{\gamma}_0\mathcal{S}\widetilde{\gamma}_0 = -\widetilde{\gamma}_0.$$

Hence the generalized 1-pdm $\widetilde{\gamma}_0$ fulfills (3.37) and the requirements of Theorem 3.65 are satisfied for the state ω_0. Therefore ω_0 is a pure quasifree state. □

An important set of states which are related to the vacuum state via a Weyl transformation is the set of coherent states. Recall that a state $\omega \in \mathcal{Z}^+$ is called coherent if there is an $f \in \mathfrak{h}$ and a Weyl transformation $\mathbb{W}_f : \mathcal{F}^+ \to \mathcal{F}^+$ such that for any $A \in \mathcal{A}^+$

$$\omega(A) = \left\langle \mathbb{W}_f^*\Omega, A\mathbb{W}_f^*\Omega \right\rangle_{\mathcal{F}}.$$

Corollary 3.68. *Eq.* (3.40) *is satisfied for every coherent state.*

Proof. For every coherent state ω we can find $\phi \in \mathfrak{h}$ such that

$$\omega(A) = \left\langle \Omega, \mathbb{W}_\phi A\mathbb{W}_\phi^*\Omega \right\rangle_{\mathcal{F}}$$

where $\mathbb{W}_\phi : \mathcal{F}^+ \to \mathcal{F}^+$ is a Weyl transformation.

We have $b = \phi$, because for any $f \in \mathfrak{h}$

$$\langle b, f\rangle_{\mathfrak{h}} = \left\langle \Omega, \mathbb{W}_\phi a^*(f)\mathbb{W}_\phi^*\Omega \right\rangle_{\mathcal{F}} = \left\langle \Omega, \left[a^*(f) + \langle\phi, f\rangle_{\mathfrak{h}}\mathbb{1}_{\mathcal{F}^+}\right]\Omega \right\rangle = \langle\phi, f\rangle_{\mathfrak{h}}$$

where we use $\langle\Omega, a^*(f)\Omega\rangle_{\mathcal{F}} = \langle a(f)\Omega, \Omega\rangle_{\mathcal{F}} = 0$. For the 1-pdm γ we find

$$\begin{aligned}\langle f, \gamma g\rangle_{\mathfrak{h}} &= \left\langle \Omega, \left[a^*(g) + \langle\phi, g\rangle_{\mathfrak{h}}\mathbb{1}_{\mathcal{F}^+}\right]\left[a(f) + \langle f, \phi\rangle_{\mathfrak{h}}\mathbb{1}_{\mathcal{F}^+}\right]\Omega \right\rangle_{\mathcal{F}} \\ &= \langle f, \phi\rangle_{\mathfrak{h}}\langle\phi, g\rangle_{\mathfrak{h}} \\ &= \langle f, b\rangle_{\mathfrak{h}}\langle b, g\rangle_{\mathfrak{h}}\end{aligned}$$

for every $f, g \in \mathfrak{h}$ and, thus, $\gamma = |b\rangle\langle b|$. Furthermore, $\alpha^* = |\overline{b}\rangle\langle b|$ by

$$\begin{aligned}\left\langle \overline{f}, \alpha^* g \right\rangle_{\mathfrak{h}} &= \left\langle \Omega, \left[a^*(g) + \langle \phi, g\rangle_{\mathfrak{h}} \mathbb{1}_{\mathcal{F}^+}\right]\left[a^*(f) + \langle \phi, f\rangle_{\mathfrak{h}} \mathbb{1}_{\mathcal{F}^+}\right]\Omega \right\rangle_{\mathcal{F}} \\ &= \langle \phi, g\rangle_{\mathfrak{h}} \langle \phi, f\rangle_{\mathfrak{h}} \\ &= \left\langle \overline{f}, \overline{b} \right\rangle_{\mathfrak{h}} \langle b, g\rangle_{\mathfrak{h}} .\end{aligned}$$

Finally we obtain

$$\mathcal{R}_b^* \widetilde{\gamma} \mathcal{R}_b = \begin{pmatrix} 0 & 0 & 0 \\ 0 & \mathbb{1}_{\mathfrak{h}} & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

which obviously fulfills (3.40′). □

5.2 Fermions

The statements of Sect. 5.1 can also be transferred to fermion systems. The fermion analogue of Lemma 3.61 is the following lemma.

Lemma 3.69. *If an operator* $\widetilde{\gamma} = \begin{pmatrix} \gamma & \alpha \\ \alpha^* & \mathbb{1}_{\mathfrak{h}} - \overline{\gamma} \end{pmatrix} : \mathfrak{h} \oplus \mathfrak{h} \to \mathfrak{h} \oplus \mathfrak{h}$ *satisfies* $0 \leq \widetilde{\gamma} \leq \mathbb{1}_{\mathfrak{h}}$, $\mathrm{tr}_{\mathfrak{h}}(\gamma) < \infty$, *and*

$$\widetilde{\gamma}^2 = \widetilde{\gamma}, \tag{3.41}$$

then there is a unique pure quasifree state $\omega \in \mathcal{Z}^-$ *that has* $\widetilde{\gamma}$ *as its generalized one-particle density matrix. Furthermore, let* $\omega \in \mathcal{Z}^-$ *be a pure quasifree state. Then the corresponding generalized one-particle density matrix* $\widetilde{\gamma}$ *fulfills* (3.41).

This lemma is a consequence of Theorems 2.3 and 2.6 of [BLS94].

Proof. From [BLS94, Theorem 2.3] we conclude that for every generalized 1-pdm $\widetilde{\gamma}$ there is a unique quasifree state $\omega \in \mathcal{Z}^-$ having $\widetilde{\gamma}$ as its generalized 1-pdm. On the one hand, [BLS94, Theorem 2.6] implies that this quasifree state is pure since the corresponding generalized 1-pdm is a projection. This proves the first assertion of the lemma.

On the other hand, [BLS94, Theorem 2.6] also states that the generalized 1-pdm of a pure quasifree state is a projection which is the second assertion and completes the proof. □

There is even a one-to-one relation between pure quasifree states and generalized 1-pdms fulfilling (3.41).

Lemma 3.70. *Let* $\omega \in \mathcal{Z}^-$. *If the generalized one-particle density matrix* $\widetilde{\gamma}$ *corresponding to the state* ω *satisfies*

$$\widetilde{\gamma}^2 = \widetilde{\gamma}, \tag{3.42}$$

then ω *is a pure quasifree state.*

Proof. Let $\mathbb{1} \equiv \mathbb{1}_{\mathfrak{h}}$ and $\widetilde{\gamma} = \left(\begin{smallmatrix} \gamma & \alpha \\ \alpha^* & \mathbb{1}-\overline{\gamma} \end{smallmatrix}\right)$ be the generalized 1-pdm of ω. Equation (3.42) implies $\alpha\overline{\gamma} = \gamma\alpha$, $\alpha^*\gamma = \overline{\gamma}\alpha^*$, $\alpha\alpha^* = \gamma - \gamma^2$, and $\alpha^*\alpha = \overline{\gamma} - \overline{\gamma}^2$. We denote by $\{\lambda_i\}_{i=1}^{\infty}$ the eigenvalues of the 1-pdm γ (counting also degeneracies) and choose the corresponding eigenfunctions $\phi_i \in \mathfrak{h}$, $i \in \mathbb{N}$, in such a way that $\{\phi_i\}_{i=1}^{\infty}$ is an ONB of the one-particle Hilbert space $\mathfrak{h}$. Furthermore let $P : \mathfrak{h} \to \mathfrak{h}$ be the orthogonal projection on the eigenspace of the eigenvalue 1 of γ and $P^{\perp} := \mathbb{1} - P$ the projection orthogonal to P. Note that both projections commute with the 1-pdm and that P is also the projection on the eigenspace of the eigenvalue 1 of $\overline{\gamma}$. From $\alpha\overline{\gamma} = \gamma\alpha$ we obtain $\alpha P\mathfrak{h} \subseteq P\mathfrak{h}$ and $\alpha P^{\perp}\mathfrak{h} \subseteq P^{\perp}\mathfrak{h}$. So P and $P^{\perp}$ commute with γ, $\overline{\gamma}$, α, and α^*.

We define $(\mathbb{1} - \gamma)^{\frac{1}{2}}$ and $(\mathbb{1} - \overline{\gamma})^{-\frac{1}{2}}\, P^{\perp}$ by

$$(\mathbb{1} - \gamma)^{\frac{1}{2}}\, \phi_i = (1 - \lambda_i)^{\frac{1}{2}}\, \phi_i \text{ and } (\mathbb{1} - \gamma)^{-\frac{1}{2}}\, P^{\perp}\phi_i = (1 - \lambda_i)^{-\frac{1}{2}}\, P^{\perp}\phi_i$$

and consider a Bogoliubov transformation $U : \mathfrak{h} \oplus \mathfrak{h} \to \mathfrak{h} \oplus \mathfrak{h}$, $U = \left(\begin{smallmatrix} u & v \\ \overline{v} & \overline{u} \end{smallmatrix}\right)$, given by

$$u := (\mathbb{1} - \gamma)^{\frac{1}{2}} \quad \text{and} \quad v := \alpha\,(\mathbb{1} - \overline{\gamma})^{-\frac{1}{2}}\, P^{\perp} + P.$$

First we show that U is indeed a Bogoliubov transformation, i.e., that (3.24a,b) hold. The operators u and v satisfy

$$\begin{aligned} uu^* + vv^* &= (\mathbb{1} - \gamma) + \left[\alpha\,(\mathbb{1} - \overline{\gamma})^{-\frac{1}{2}}\, P^{\perp} + P\right]\left[(\mathbb{1} - \overline{\gamma})^{-\frac{1}{2}}\, P^{\perp}\alpha^* + P\right] \\ &= \mathbb{1} - \gamma + \alpha\,(\mathbb{1} - \overline{\gamma})^{-1}\, P^{\perp}\alpha^* + P + \alpha\,(\mathbb{1} - \overline{\gamma})^{-\frac{1}{2}}\, P^{\perp}P \\ &\qquad + P\,(\mathbb{1} - \overline{\gamma})^{-\frac{1}{2}}\, P^{\perp}\alpha^*. \end{aligned}$$

With $\alpha^*\gamma = \overline{\gamma}\alpha^*$ and $\alpha\alpha^* = \gamma - \gamma^2$ we have

$$uu^* + vv^* = \mathbb{1} - \gamma + \alpha\alpha^*\,(\mathbb{1} - \gamma)^{-1}\, P^{\perp} + \gamma P = \mathbb{1}.$$

$u^*u + v^T\overline{v} = \mathbb{1}$ can be shown analogously. Moreover, using $(\mathbb{1} - \gamma)^{\frac{1}{2}}\, P = 0$ and $(\mathbb{1} - \overline{\gamma})^{\frac{1}{2}}\, P = 0$,

$$\begin{aligned} u^*v + v^T\overline{u} &= (\mathbb{1} - \gamma)^{\frac{1}{2}}\left[\alpha\,(\mathbb{1} - \overline{\gamma})^{-\frac{1}{2}}\, P^{\perp} + P\right] \\ &\qquad + \left[(\mathbb{1} - \overline{\gamma})^{-\frac{1}{2}}\, P^{\perp}\alpha^T + P\right](\mathbb{1} - \overline{\gamma})^{\frac{1}{2}} \\ &= \alpha\, P^{\perp} + (\mathbb{1} - \gamma)^{\frac{1}{2}}\, P - P^{\perp}\alpha + P\,(\mathbb{1} - \overline{\gamma})^{\frac{1}{2}} \\ &= 0. \end{aligned}$$

$uv^T + vu^T = 0$ is obtained similarly. Since furthermore the (operator valued) entries on the diagonal of the matrix U and, due to $\alpha^* = -\overline{\alpha}$, those on the off-diagonal as well are complex conjugate to each other, U is a fermion Bogoliubov transformation according to Definition 3.33.

The Bogoliubov transformation U has a unitary representation $\mathbb{U}$ because

$$\begin{aligned} \mathrm{tr}_{\mathfrak{h}}(v^*v) &= \mathrm{tr}_{\mathfrak{h}}\Big(\left[(\mathbb{1} - \overline{\gamma})^{-\frac{1}{2}}\, P^{\perp}\alpha^* + P\right]\left[\alpha\,(\mathbb{1} - \overline{\gamma})^{-\frac{1}{2}}\, P^{\perp} + P\right]\Big) \\ &= \mathrm{tr}_{\mathfrak{h}}\big((\mathbb{1} - \overline{\gamma})^{-\frac{1}{2}}\,\overline{\gamma}\,(\mathbb{1} - \overline{\gamma})\,(\mathbb{1} - \overline{\gamma})^{-\frac{1}{2}}\, P^{\perp} + P\big) \end{aligned}$$

due to $\alpha^*\alpha = \overline{\gamma} - \overline{\gamma}^2$ and, thus,

$$\mathrm{tr}_{\mathfrak{h}}(v^* v) = \mathrm{tr}_{\mathfrak{h}}(\overline{\gamma} P^{\perp} + P) = \mathrm{tr}_{\mathfrak{h}}(\gamma) = \omega(\widehat{\mathbb{N}}) < \infty.$$

We define a state $\omega_U \in \mathcal{Z}^-$ by $\omega_U(A) := \omega\big(\mathbb{U} A \mathbb{U}^*\big)$ for any $A \in \mathcal{A}^-$ and denote its density matrix by ρ_U. We show that the corresponding generalized 1-pdm $\widetilde{\gamma}_U$ is given by

$$\widetilde{\gamma}_U = \begin{pmatrix} 0 & 0 \\ 0 & \mathbb{1} \end{pmatrix}.$$

Consequently

$$\gamma_U = 0 \tag{3.43}$$

and the transformed generalized 1-pdm $\widetilde{\gamma}_U$ is a projection.

By Lemma 3.47 the Bogoliubov transformation U yields $\widetilde{\gamma}_U = U^* \widetilde{\gamma} U$. So U satisfies

$$\widetilde{\gamma} = U \begin{pmatrix} 0 & 0 \\ 0 & \mathbb{1} \end{pmatrix} U^* = \begin{pmatrix} vv^* & vu^T \\ \overline{u}v^* & \overline{u}u^T \end{pmatrix}$$

that is $\gamma = vv^*$ and $\alpha = vu^T$. This is indeed the case since

$$vv^* = P + \alpha \left(\mathbb{1} - \overline{\gamma}\right)^{-1} P^{\perp} \alpha^* = \gamma P + \alpha\alpha^* \left(\mathbb{1} - \gamma\right)^{-1} P^{\perp} = \gamma P + \gamma P^{\perp} = \gamma,$$
$$vu^T = \alpha \left(\mathbb{1} - \overline{\gamma}\right)^{-\frac{1}{2}} P^{\perp} \left(\mathbb{1} - \overline{\gamma}\right)^{\frac{1}{2}} + \alpha \left(\mathbb{1} - \overline{\gamma}\right)^{-\frac{1}{2}} P^{\perp} P = \alpha P^{\perp} = \alpha.$$

Here we used $\alpha P = 0$ which follows from $P\alpha^*\alpha P = P\left(\overline{\gamma} - \overline{\gamma}^2\right) P = 0$.

Let $\{\varphi_n\}_{n=1}^{\infty}$ denote an arbitrary ONB of $\mathfrak{h}$. We define

$$\mathcal{K} := \left\{ k \in \mathbb{N} \to \{0,1\} \,\middle|\, \exists n_0 \in \mathbb{N} \text{ s.t. } \forall n \geq n_0 : k_n = 0 \right\}.$$

The elements $K \in \mathcal{K}$ form the occupancy number representation of the fermion Fock space. If we define

$$c_K^* := \prod_{\substack{n=1 \\ K_n \neq 0}}^{\infty} c_n^*$$

for any $K \in \mathcal{K}$, the functions $\Psi_{(0,0,\dots)} = \Omega$ and $\Psi_K \in \mathcal{F}^-$ given by $\Psi_K := c_K^* \Omega$ for $K \in \mathcal{K}$, $K \neq (0,0,\dots)$, form an ONB of the fermion Fock space. Furthermore for any $n \in \mathbb{N}$ and any $K \in \mathcal{K}$ with $K_n = 1$ we write $K \setminus \{n\}$ for the set where the particle in the state given by φ_n is removed, but the others are left unchanged. Now we write the density matrix corresponding to ω_U as

$$\rho_U = \sum_{K,L \in \mathcal{K}} \mu_{K,L} \left|\Psi_K\right\rangle \left\langle \Psi_L\right|$$

where the coefficients are given by $\mu_{K,L} := \omega_U\big(\left|\Psi_L\right\rangle \left\langle \Psi_K\right|\big) \in \mathbb{C}$ for any sets $K, L \in \mathcal{K}$. Applying the Cauchy–Schwarz inequality, we obtain for every $n \in \mathbb{N}$ and every pair $K, L \in \mathcal{K}$ with $K_n = 1$

$$\begin{aligned} |\mu_{K,L}|^2 &= |\omega_U\big(c_L^* \left|\Omega\right\rangle \left\langle \Omega\right| c_{K\setminus\{n\}} c_n\big)|^2 \\ &\leq \omega_U\big(c_L^* \left|\Omega\right\rangle \left\langle \Omega, c_{K\setminus\{n\}} c_{K\setminus\{n\}}^* \Omega \right\rangle_{\mathfrak{h}} \left\langle \Omega\right| c_L\big) \omega_U\big(c_n^* c_n\big). \end{aligned}$$

By (3.43) $\omega_U\big(c_n^* c_n\big) = \langle \varphi_n, \gamma_U \varphi_n \rangle_{\mathfrak{h}} = 0$ for every $n \in \mathbb{N}$ and $\mu_{K,L} = 0$ if one of the sets $K, L \in \mathcal{K}$ is not $(0, 0, \dots)$. Hence for any $A \in \mathcal{A}^-$

$$\omega_U(A) = \langle \Omega, A\Omega \rangle_{\mathcal{F}}.$$

Since U is a Bogoliubov transformation with unitary implementation $\mathbb{U}$ and invertible, we obtain for any $A \in \mathcal{A}^-$

$$\omega(A) = \omega_U\big(\mathbb{U}^* A \mathbb{U}\big) = \langle \mathbb{U}\Omega, A\mathbb{U}\Omega \rangle_{\mathcal{F}}.$$

Therefore the state ω is pure and quasifree by Remark 3.39 which yields the assertion. □

From the last two lemmas we conclude:

Theorem 3.71. *Let $\omega \in \mathcal{Z}^-$ be a state. Then the following statements are equivalent:*

(i) *ω is a pure quasifree state.*

(ii) *The generalized* 1*-pdm $\widetilde{\gamma}$ of the state ω satisfies*

$$\widetilde{\gamma}^2 = \widetilde{\gamma}.$$

Proof. The implication $(i) \Rightarrow (ii)$ is given by the second assertion of Lemma 3.69 and the reverse by Lemma 3.70. □

Chapter **4**

Fermion Correlation Inequalities Derived from G- and P-Conditions

The following sections are a revised version of an article with Volker Bach and Edmund Menge, which was published in Documenta Mathematica in 2012, [BKM12].

1 Introduction

The dynamics of N electrons in an atom ($K = 1$) or molecule ($K \geq 2$) with K nuclei of charges $\underline{Z} := (Z_1, Z_2, \dots, Z_K)$ fixed at positions $\underline{R} := (R_1, R_2, \dots, R_K)$ is generated by the Hamiltonian

$$H^{(N)}(\underline{Z}, \underline{R}) := \sum_{n=1}^{N} \left(-\Delta_{x_n} - \sum_{j=1}^{K} \frac{Z_j}{|x_n - R_j|} \right) + \sum_{1 \leq n < m \leq N} \frac{1}{|x_n - x_m|} \quad (4.1)$$

to lowest order in the Born–Oppenheimer approximation. $H^{(N)}(\underline{Z}, \underline{R}) \equiv H^{(N)}$ is a selfadjoint operator which is bounded below and defined on a suitable dense domain $\mathcal{D}^{(N)}$ in the N-particle Fock space $\mathfrak{h}^{\wedge N}$ of antisymmetric N-electron wave functions, cf. (2.4) below.

Basic quantities of interest are the ground state energy

$$E_{\text{gs}}(N, \underline{Z}, \underline{R}) := \inf \left\{ \sigma \left\{ H^{(N)}(\underline{Z}, \underline{R}) \right\} \right\}$$

whose variational characterization

$$\begin{aligned} &E_{\text{gs}}(N, \underline{Z}, \underline{R}) \\ &\quad = \inf \left\{ \left\langle \Psi^{(N)}, H^{(N)} \Psi^{(N)} \right\rangle \,\middle|\, \Psi^{(N)} \in \mathcal{D}^{(N)} \cap \mathfrak{h}^{\wedge N},\ \|\Psi^{(N)}\| = 1 \right\} \end{aligned} \quad (4.2)$$

is given by the Rayleigh–Ritz principle and the corresponding ground states $\Psi^{(N)}_{\text{gs}}$, i.e., normalized solutions of the stationary Schrödinger equation

$$H^{(N)}(\underline{Z}, \underline{R})\, \Psi_{\mathrm{gs}}^{(N)} \;=\; E_{\mathrm{gs}}(N, \underline{Z}, \underline{R})\, \Psi_{\mathrm{gs}}^{(N)}.$$

The Hartree–Fock (HF) variational principle is an important method to obtain approximations to both, the ground state energy and ground states. The HF energy $E_{\mathrm{hf}}(N, \underline{Z}, \underline{R})$ is defined by restricting the variation in (4.2) to $SD^{(N)}$,

$$\begin{aligned} & E_{\mathrm{hf}}(N, \underline{Z}, \underline{R}) \\ & \quad = \inf \Big\{ \Big\langle \Phi^{(N)}, H^{(N)} \Phi^{(N)} \Big\rangle \,\Big|\, \Phi^{(N)} \in \mathcal{D}^{(N)} \cap SD^{(N)},\ \|\Phi^{(N)}\| = 1 \Big\} \end{aligned} \tag{4.3}$$

where $SD^{(N)} \subseteq \mathfrak{h}^{\wedge N}$ denotes the set of Slater determinants, i.e., the set of all antisymmetrized product vectors $\varphi_1 \wedge \cdots \wedge \varphi_N$. Since the variation in (4.3), compared to (4.2), is restricted, we clearly have

$$E_{\mathrm{hf}}(N, \underline{Z}, \underline{R}) \;\geq\; E_{\mathrm{gs}}(N, \underline{Z}, \underline{R}).$$

A lower bound to the ground state energy by the HF energy minus an error which is small in the large-Z limit was obtained by one of us in [Bac92, Bac93]. In the case of a neutral atom, i.e., $N = Z := Z_1$ and $R_1 = 0$, the resulting estimate was

$$E_{\mathrm{gs}}(Z) \;\geq\; E_{\mathrm{hf}}(Z) - \mathcal{O}\big(Z^{(5/3)-\epsilon}\big) \tag{4.4}$$

for some $\epsilon > 0$. The error term $\mathcal{O}(Z^{(5/3)-\epsilon})$ is small compared to all three contributions to $E_{\mathrm{hf}}(Z)$, namely, the kinetic, the classical electrostatic, and the exchange energy which are at least of size $cZ^{5/3}$ in magnitude for some constant $c > 0$.

A key inequality derived in [Bac92] that eventually lead to (4.4) is the fermion correlation estimate

$$\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}} \Big((X \otimes X) \Gamma^{(\mathrm{T})} \Big) \;\geq\; -\,\mathrm{tr}_{\mathfrak{h}}\,(X\gamma) \min \Big\{ 1;\ \mathrm{const} \cdot \sqrt{\mathrm{tr}_{\mathfrak{h}}\,(X\,(\gamma - \gamma^2))} \Big\} \tag{4.5}$$

where $X = X^* = X^2$ is an orthogonal projection, $\Gamma^{(\mathrm{T})} := \Gamma - (\mathbb{1}_{\mathfrak{h}\otimes\mathfrak{h}} - \mathrm{Ex})(\gamma \otimes \gamma)$, $\Gamma \equiv \Gamma_{\Phi^{(N)}}$ is the two-particle, and $\gamma \equiv \gamma_{\Phi^{(N)}}$ the one-particle density matrix of a normalized N-electron state $\Phi^{(N)} \in \mathfrak{h}^{\wedge N}$.

The purpose of the present paper is to give an alternative derivation of (4.5) by using ideas originating from the theory of N-representability. More precisely, we show that (4.5) follows already from the G-condition and the P-condition specified by Garrod and Percus [GP64] and Coleman [Col63].

Observing that the Rayleigh–Ritz principle (4.2) can be rewritten as a variation over all N-representable two-particle density matrices Γ, we consequently obtain (4.4) from relaxing the requirement of N-representability of Γ to merely requiring Γ to fulfill the G-condition and the P-condition:

Theorem 4.1 (Main Theorem). *The G- and the P-condition imply* (4.5).

We note that (4.5) was also derived by Graf and Solovej in [GS94] by a different method that, in retrospective, resembles the application of Garrod and Percus' G-condition. In fact, one part of the derivation in [GS94] follows already from the G-condition. A main difference to using representability methods, however, lies in the use of operator inequalities in [GS94] which are necessarily formulated on the N-particle Hilbert space, as opposed to the one- or two-particle Hilbert spaces in the presented work.

In future work we plan to sharpen this result by making additional use of Erdahl's T_1- and T_2-conditions [Erd78b, Erd78a] which have recently lead to very good numerical results in quantum chemistry computations [CLS06, ME01, NAHM11], as well as Coleman's Q-condition which was also given in [Col63] but is not necessary for the derivation of our present result. Furthermore, similar representability conditions also exist for bosons [ME01]. There we like to address the question whether analogous results can also be obtained.

2 Density Matrices and Reduced Density Matrices

2.1 Fock Space, Creation and Annihilation Operators

Let $\mathfrak{h}$ be a separable complex Hilbert space which we henceforth refer to as the one-particle Hilbert space. The fermion Fock space $\mathcal{F}^-$ is defined to be the orthogonal sum

$$\mathcal{F}^- := \bigoplus_{N=0}^{\infty} \mathfrak{h}^{\wedge N}$$

where

$$\mathfrak{h}^{\wedge N} := A_N\Big(\bigotimes^N \mathfrak{h}\Big)$$

is the antisymmetric tensor product of N copies of $\mathfrak{h}$ for $N \geq 1$ and $\mathfrak{h}^{\wedge 0} := \mathbb{C}$. The vacuum vector Ω is the normalized basis vector of $\mathfrak{h}^{\wedge 0}$. Here, A_N is the orthogonal projection from $\bigotimes^N \mathfrak{h}$ onto $\mathfrak{h}^{\wedge N}$ uniquely defined by

$$\begin{aligned} A_N\left(\varphi_1 \otimes \cdots \otimes \varphi_N\right) &:= \frac{1}{N!} \sum_{\pi \in \mathcal{S}_N} (-1)^\pi \, \varphi_{\pi(1)} \otimes \cdots \otimes \varphi_{\pi(N)} \\ &=: \frac{1}{\sqrt{N!}} \varphi_1 \wedge \cdots \wedge \varphi_N \end{aligned}$$

for $\varphi_1, \ldots, \varphi_N \in \mathfrak{h}$. It is convenient to introduce creation operators $c^*(f) \in \mathcal{B}(\mathcal{F}^-)$ for any $f \in \mathfrak{h}$ by

$$c^*(f)\Omega := f, \tag{4.6}$$

$$c^*(f)\left(\varphi_1 \wedge \cdots \wedge \varphi_N\right) := f \wedge \varphi_1 \wedge \cdots \wedge \varphi_N \tag{4.7}$$

for $\varphi_1, \dots, \varphi_N \in \mathfrak{h}$ and extension by linearity and continuity. By induction and (4.6)-(4.7)

$$\varphi_1 \wedge \varphi_2 \wedge \cdots \wedge \varphi_N = c^*(\varphi_1)c^*(\varphi_2)\cdots c^*(\varphi_N)\Omega$$

for all $\varphi_1, \varphi_2, \dots, \varphi_N \in \mathfrak{h}$. If $\{\varphi_k\}_{k=1}^{\infty}$ is an orthonormal basis (ONB) of $\mathfrak{h}$, then for any $N \in \mathbb{N}$

$$\left\{c^*(\varphi_{k_1})\cdots c^*(\varphi_{k_N})\Omega \,\middle|\, 1 \le k_1 < k_2 < \cdots < k_N\right\}$$

is an ONB of $\mathfrak{h}^{\wedge N}$ and

$$\left\{c^*(\varphi_{k_1})\cdots c^*(\varphi_{k_N})\Omega \,\middle|\, N \in \mathbb{N}_0,\ 1 \le k_1 < k_2 < \cdots < k_N\right\} \tag{4.8}$$

is an ONB of $\mathcal{F}^-$.
The adjoint operators $c(f) := (c^*(f))^* \in \mathcal{B}(\mathcal{F}^-)$ with $f \in \mathfrak{h}$ are the annihilation operators. Note that, while $f \mapsto c^*(f)$ is linear, $f \mapsto c(f)$ is antilinear. Together with the creation operators they fulfill the canonical anticommutation relations (CAR), i.e.,

$$\{c(f), c^*(g)\} = \langle f, g\rangle_{\mathfrak{h}}\, \mathbb{1}_{\mathcal{F}} \quad , \quad \{c^*(f), c^*(g)\} = 0 \tag{4.9}$$

for all $f, g \in \mathfrak{h}$ where $\{A, B\} := AB + BA$ denotes the anticommutator.
Moreover,

$$c(f)\Omega = 0, \tag{4.10}$$

for all $f \in \mathfrak{h}$ and $\left\{c^*(f), c(f) \,\middle|\, f \in \mathfrak{h}\right\}$ is completely determined by (4.6), (4.9), and (4.10), i.e., (4.7)-(4.8) follow from (4.6), (4.9), and (4.10). The creation and annihilation operators introduced here are a specific representation of the (abstract) CAR (4.9), namely the Fock representation. For φ_k being an arbitrary element of a given ONB $\{\varphi_k\}_{k=1}^{\infty}$ of $\mathfrak{h}$ we write

$$c_k^* \equiv c^*(\varphi_k),\ c_k \equiv c(\varphi_k).$$

An important unbounded, selfadjoint, and positive semi-definite operator on $\mathcal{F}^-$ is the number operator $\widehat{\mathbb{N}}$ defined by

$$\widehat{\mathbb{N}}\left(c^*(f_1)\cdots c^*(f_N)\Omega\right) := N \cdot c^*(f_1)\cdots c^*(f_N)\Omega$$

for any $f_1, \dots, f_N \in \mathfrak{h}$. It is not difficult to see that

$$\widehat{\mathbb{N}} = \sum_{k=1}^{\infty} c_k^* c_k$$

as a quadratic form for any ONB $\{\varphi_k\}_{k=1}^{\infty}$ of $\mathfrak{h}$.

2.2 Density Matrices

A positive trace class operator $\rho \in \mathcal{L}^1_+(\mathcal{F}^-)$ of unit trace, $\mathrm{tr}_{\mathcal{F}}(\rho) = 1$, is called density matrix. Given a density matrix ρ, the map $A \mapsto \mathrm{tr}_{\mathcal{F}}(\rho A)$ defines a state, i.e., a normalized, linear, and positive functional on $\mathcal{B}(\mathcal{F}^-) \ni A$. If $\Psi \in \mathcal{F}^-$ is a normalized vector, then $|\Psi\rangle\langle\Psi|$ is a density matrix (of rank one) called pure state. In this paper we study fermion systems with a repulsive interaction and whose dynamics preserve the particle number. For this reason we restrict our attention to density matrices which commute with the particle number operator and have a finite squared particle number expectation value:

$$\rho = \bigoplus_{N=0}^{\infty} \rho^{(N)} \quad \text{and} \quad \left\langle \widehat{\mathbb{N}}^2 \right\rangle_\rho < \infty \tag{4.11}$$

where here and henceforth we denote for any $A \in \mathcal{B}(\mathfrak{h})$

$$\langle A \rangle_\rho := \mathrm{tr}_{\mathcal{F}} \left(\rho^{\frac{1}{2}} A \rho^{\frac{1}{2}} \right).$$

Note that for any choice of $f_1, \ldots, f_m, g_1, \ldots, g_n \in \mathfrak{h}$ with $m, n \in \mathbb{N} \cup \{0\}$, $m \neq n$, $\mathrm{tr}_{\mathcal{F}^-}(\rho\, c^*(f_1) \cdots c^*(f_m) c(g_1) \cdots c(g_n)) = 0$ due to (4.11).

2.3 Reduced Density Matrices

Given a density matrix $\rho \in \mathcal{L}^1_+(\mathcal{F}^-)$ subject to (4.11), we introduce two bounded operators, $\gamma_\rho \in \mathcal{B}(\mathfrak{h})$ and $\Gamma_\rho \in \mathcal{B}(\mathfrak{h} \otimes \mathfrak{h})$, by

$$\langle f, \gamma_\rho g \rangle_{\mathfrak{h}} := \mathrm{tr}_{\mathcal{F}}(\rho\, c^*(g) c(f)) \tag{4.12}$$

for all $f, g \in \mathfrak{h}$ and for all $f_1, f_2, g_1, g_2 \in \mathfrak{h}$

$$\langle f_1 \otimes f_2, \Gamma_\rho (g_1 \otimes g_2) \rangle_{\mathfrak{h} \otimes \mathfrak{h}} := \mathrm{tr}_{\mathcal{F}}(\rho\, c^*(g_2) c^*(g_1) c(f_1) c(f_2)). \tag{4.13}$$

γ_ρ is called the one-particle density matrix (1-pdm) and Γ_ρ the two-particle density matrix (2-pdm) corresponding to ρ. For an arbitrary ONB $\{\varphi_k\}_{k=1}^\infty$ of $\mathfrak{h}$ we define the exchange operator $\mathrm{Ex} \in \mathcal{B}(\mathfrak{h} \otimes \mathfrak{h})$ by

$$\mathrm{Ex} := \sum_{k,l=1}^{\infty} |\varphi_k \otimes \varphi_l\rangle \langle \varphi_l \otimes \varphi_k|,$$

such that $\mathrm{Ex}(f \otimes g) = g \otimes f$. Then the CAR lead to the antisymmetry property of Γ_ρ:

$$\mathrm{Ex}\, \Gamma_\rho = -\Gamma_\rho = \Gamma_\rho\, \mathrm{Ex}.$$

Furthermore, we define

$$\Gamma_{kl;mn} := \langle \varphi_k \otimes \varphi_l, \Gamma(\varphi_m \otimes \varphi_n) \rangle_{\mathfrak{h} \otimes \mathfrak{h}}.$$

By the definition of Γ_ρ we have $\Gamma_{kl;mn} = -\Gamma_{lk;mn} = \Gamma_{lk;mn}$.

The following properties of the 1-pdm and the 2-pdm are easily proven:

Lemma 4.2. *Let $\rho \in \mathcal{L}^1_+(\mathcal{F}^-)$ be a density matrix obeying (4.11). Then the following assertions hold true:*

i) $\gamma_\rho \in \mathcal{L}^1_+(\mathfrak{h})$, $\quad 0 \le \gamma_\rho \le \mathbb{1}_\mathfrak{h}$, $\quad \mathrm{tr}_\mathfrak{h}(\gamma_\rho) = \left\langle \widehat{\mathbb{N}} \right\rangle_\rho$, $\quad \Gamma_\rho \in \mathcal{L}^1_+(\mathfrak{h} \otimes \mathfrak{h})$, $0 \le \Gamma_\rho \le \left\langle \widehat{\mathbb{N}} \right\rangle_\rho \mathbb{1}_{\mathfrak{h}\otimes\mathfrak{h}}$, *and* $\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}(\Gamma_\rho) = \left\langle \widehat{\mathbb{N}} \left(\widehat{\mathbb{N}} - \mathbb{1}_\mathcal{F} \right) \right\rangle_\rho$.

ii) If $\mathrm{ran}(\rho) \subseteq \mathfrak{h}^{\wedge N}$, *then for all* $f, g \in \mathfrak{h}$

$$\langle f, \gamma_\rho g \rangle_\mathfrak{h} = \frac{1}{N-1} \sum_{k=1}^{\infty} \langle f \otimes \varphi_k, \Gamma_\rho (g \otimes \varphi_k) \rangle_{\mathfrak{h}\otimes\mathfrak{h}},$$

where $\{\varphi_k\}_{k=1}^\infty$ *is an ONB of* $\mathfrak{h}$.

iii) Furthermore,

$$\rho = |f c(\varphi_1) \cdots c^*(\varphi_N)\Omega\rangle \langle c^*(\varphi_1) \cdots c^*(\varphi_N)\Omega| \ \Leftrightarrow\ \gamma_\rho = \sum_{i=1}^{N} |\varphi_i\rangle \langle \varphi_i|$$

and in this case

$$\Gamma_\rho = (\mathbb{1}_{\mathfrak{h}\otimes\mathfrak{h}} - \mathrm{Ex}) (\gamma_\rho \otimes \gamma_\rho).$$

2.4 Hamiltonian and the Ground State Energy

Recall from (4.1) that the Hamiltonian of an atom or molecule is given by

$$H^{(N)}(\underline{Z}, \underline{R}) := \sum_{n=1}^{N} \left(-\Delta_{x_n} - \sum_{k=1}^{K} \frac{Z_k}{|x_n - R_k|} \right) + \sum_{1 \le n < m \le N} \frac{1}{|x_n - x_m|}.$$

Choosing an ONB $\{\varphi_k\}_{k=1}^\infty$ of $\mathfrak{h} = \mathrm{L}^2(\mathbb{R}^3 \times \mathbb{Z}_2)$ such that $\{\varphi_k\}_{k=1}^\infty \subseteq \mathrm{H}^2(\mathbb{R}^3 \times \mathbb{Z}_2)$ where $\mathrm{H}^2(\mathbb{R}^3 \times \mathbb{Z}_2)$ denotes the Sobolev space, we define

$$h_{kl} := \left\langle \varphi_k, \left(-\Delta_x - \sum_{k=1}^{K} \frac{Z_k}{|x - R_k|} \right) \varphi_l \right\rangle_\mathfrak{h},$$

$$V_{kl;mn} := \left\langle \varphi_k \otimes \varphi_l, \frac{1}{|x-y|} (\varphi_m \otimes \varphi_n) \right\rangle_{\mathfrak{h}\otimes\mathfrak{h}},$$

and

$$\mathbb{H} := \sum_{k,l=1}^{\infty} h_{kl}\, c_k^* c_l + \sum_{k,l,m,n=1}^{\infty} V_{kl;mn}\, c_l^* c_k^* c_m c_n.$$

Stability of matter ensures that $\mathbb{H} + \mu\widehat{\mathbb{N}}$ is selfadjoint and bounded below provided $\mu < \infty$ is sufficiently large. Moreover, the Hamiltonian of an atom or molecule can be viewed as

$$H^{(N)}(\underline{Z}, \underline{R}) = \mathbb{H}\big|_{\mathfrak{h}^{\wedge N}},$$

i.e., $H^{(N)}(\underline{Z}, \underline{R})$ is the restriction of $\mathbb{H}$ to $\mathfrak{h}^{\wedge N}$.

The ground state energy $E_{gs} \equiv E_{gs}(N, \underline{Z}, \underline{R})$ can now be reexpressed as

$$E_{gs} = \inf\left\{ \mathrm{tr}_{\mathcal{F}}\left(\rho^{\frac{1}{2}} \mathbb{H} \rho^{\frac{1}{2}}\right) \,\middle|\, \rho \in \mathcal{L}^1_+(\mathcal{F}^-),\ \widehat{\mathbb{N}}\rho = N\rho,\ \mathrm{tr}_{\mathcal{F}}(\rho) = 1 \right\}$$
$$= \inf\left\{ \mathcal{E}\left(\gamma_\rho, \Gamma_\rho\right) \,\middle|\, \rho \in \mathcal{L}^1_+(\mathcal{F}^-),\ \widehat{\mathbb{N}}\rho = N\rho,\ \mathrm{tr}_{\mathcal{F}}(\rho) = 1 \right\}$$

where the energy functional is defined as

$$\mathcal{E}\left(\gamma_\rho, \Gamma_\rho\right) := \mathrm{tr}_{\mathfrak{h}}\left(h\gamma_\rho\right) + \frac{1}{2}\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(V\Gamma_\rho\right).$$

We call $(\gamma, \Gamma) \in \mathcal{B}(\mathfrak{h}) \times \mathcal{B}(\mathfrak{h} \otimes \mathfrak{h})$ *N-representable* if there exists a density matrix $\rho \in \mathcal{L}^1_+(\mathcal{F}^-)$ with $\widehat{\mathbb{N}}\rho = N\rho$ and $\mathrm{tr}_{\mathcal{F}}(\rho) = 1$ such that $\gamma = \gamma_\rho$ and $\Gamma = \Gamma_\rho$. Using the notion of N-representability, the ground state energy can be rewritten as

$$E_{gs} = \inf\left\{ \mathcal{E}(\gamma, \Gamma) \,\middle|\, (\gamma, \Gamma) \text{ is } N\text{-representable} \right\}.$$

By Lemma 4.2 we have that

$$E_{hf} = \inf\left\{ \mathcal{E}\Big(\gamma, (\mathbb{1}_{\mathfrak{h}\otimes\mathfrak{h}} - \mathrm{Ex})(\gamma\otimes\gamma)\Big) \,\middle|\, \gamma = \gamma^* = \gamma^2,\ \mathrm{tr}_{\mathfrak{h}}(\gamma) = N \right\},$$

and Lieb's variational principle [Lie81, Bac92] ensures that actually

$$E_{hf} = \inf\left\{ \mathcal{E}\Big(\gamma, (\mathbb{1}_{\mathfrak{h}\otimes\mathfrak{h}} - \mathrm{Ex})(\gamma\otimes\gamma)\Big) \,\middle|\, 0 \le \gamma \le \mathbb{1}_{\mathfrak{h}},\ \mathrm{tr}_{\mathfrak{h}}(\gamma) = N \right\}.$$

3 G-, P-, and Q-Conditions

In this section we derive necessary conditions on (γ, Γ) to be N-representable. To this end we assume $N \in \mathbb{N}$, $\gamma \in \mathcal{L}^1(\mathfrak{h})$ with $0 \le \gamma \le \mathbb{1}_{\mathfrak{h}}$, and $\mathrm{tr}_{\mathfrak{h}}(\gamma) = N$, $\Gamma \in \mathcal{L}^1(\mathfrak{h}\otimes\mathfrak{h})$, $\mathrm{Ex}\,\Gamma = \Gamma\,\mathrm{Ex} = -\Gamma$, and we call (γ, Γ) admissible in this case.

(P) (γ, Γ) fulfills the P-condition

$$:\Leftrightarrow \Gamma \ge 0.$$

(G) (γ, Γ) fulfills the G-condition

$$:\Leftrightarrow \forall A \in \mathcal{B}(\mathfrak{h}) :\ \mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left((A^*\otimes A)\left(\Gamma + \mathrm{Ex}\left(\gamma\otimes\mathbb{1}_{\mathfrak{h}}\right)\right)\right) \ge \left|\mathrm{tr}_{\mathfrak{h}}\left(A\gamma\right)\right|^2. \tag{4.14}$$

(Q) (γ, Γ) fulfills the Q-condition

$$:\Leftrightarrow \Gamma + (\mathbb{1}_{\mathfrak{h}\otimes\mathfrak{h}} - \mathrm{Ex})(\mathbb{1}_{\mathfrak{h}}\otimes\mathbb{1}_{\mathfrak{h}} - \gamma\otimes\mathbb{1}_{\mathfrak{h}} - \mathbb{1}_{\mathfrak{h}}\otimes\gamma) \ge 0.$$

Our main result of this section is

Theorem 4.3. *Let $\rho \in \mathcal{L}^1(\mathcal{F}^-)$ (not necessarily positive) such that $\mathrm{tr}_{\mathcal{F}}(\rho) = 1$, $\mathrm{tr}_{\mathcal{F}}\left(|\rho|^{\frac{1}{2}}\,\widehat{\mathbb{N}}^2\,|\rho|^{\frac{1}{2}}\right) < \infty$, and that ρ preserves the particle number, i.e., $\left[\widehat{\mathbb{N}}, \rho\right] = 0$. Define γ_ρ and Γ_ρ by (4.12) and (4.13), respectively, and let $\{\varphi_k\}_{k=1}^\infty$ be an ONB of $\mathfrak{h}$. Then the following two statements are equivalent:*

(i) If $\mathcal{P}_r \in \mathcal{B}(\mathcal{F}^-)$ *is a polynomial in* $\{c_k^*, c_k\}_{k=1}^\infty$ *of degree* $r \leq 2$*, then*

$$\mathrm{tr}_{\mathcal{F}} \left(\rho \, \mathcal{P}_r^* \mathcal{P}_r\right) \geq 0.$$

(ii) $\left(\gamma_\rho, \Gamma_\rho\right)$ *is admissible and fulfills the G-, P-, and Q-conditions.*

Before we turn to the proof of Theorem 4.3, we establish its finite-dimensional analogue in Lemma 4.4 below. Theorem 4.3 then follows from Lemma 4.4 by a limiting argument.

Lemma 4.4. *Let* $\rho \in \mathcal{L}^1(\mathcal{F}^-)$ *(not necessarily positive) such that* $\mathrm{tr}_{\mathcal{F}}(\rho) = 1$, $\mathrm{tr}_{\mathcal{F}}\left(|\rho|^{\frac{1}{2}}\, \widehat{\mathbb{N}}^2\, |\rho|^{\frac{1}{2}}\right) < \infty$*, and that* ρ *preserves the particle number, i.e.,* $\left[\widehat{\mathbb{N}}, \rho\right] = 0$*. Define* γ_ρ *and* Γ_ρ *by* (4.12) *and* (4.13)*, respectively, and let* $\{\varphi_k\}_{k=1}^\infty$ *be an ONB of* $\mathfrak{h}$*. Then the following statements are equivalent:*

(i) If $\mathcal{P}_r \in \mathcal{B}(\mathcal{F}^-)$ *is a polynomial in* $\{c_k^*, c_k\}_{k=1}^\infty$ *of degree* $r \leq 2$*, then*

$$\mathrm{tr}_{\mathcal{F}} \left(\rho \, \mathcal{P}_r^* \mathcal{P}_r\right) \geq 0. \tag{4.15}$$

(ii) For any $\phi \in \mathrm{span}\{\varphi_k |\, k \in \mathbb{N}\}$ *and* $\Psi \in \mathrm{span}\{\varphi_k \otimes \varphi_l |\, k, l \in \mathbb{N}\}$ *we have*

$$0 \leq \langle \phi, \gamma_\rho \phi \rangle_{\mathfrak{h}} \leq 1, \tag{4.16}$$

$$\langle \Psi, \Gamma_\rho \Psi \rangle_{\mathfrak{h}\otimes\mathfrak{h}} \geq 0, \tag{4.17}$$

$$\left\langle \Psi, \left(\Gamma_\rho + (\mathbb{1}_{\mathfrak{h}\otimes\mathfrak{h}} - \mathrm{Ex})(\mathbb{1}_{\mathfrak{h}} \otimes \mathbb{1}_{\mathfrak{h}} - \gamma_\rho \otimes \mathbb{1}_{\mathfrak{h}} - \mathbb{1}_{\mathfrak{h}} \otimes \gamma_\rho)\right) \Psi \right\rangle_{\mathfrak{h}\otimes\mathfrak{h}} \geq 0, \tag{4.18}$$

and for all $A := \sum_{k,l=1}^M \alpha_{kl} \, |\varphi_k\rangle \langle \varphi_l|$, $M < \infty$, $(\alpha_{kl})_{k,l=1}^M \in \mathbb{C}^{M\times M}$,

$$\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}} \left((A^* \otimes A) \left(\Gamma_\rho + \mathrm{Ex}\left(\gamma_\rho \otimes \mathbb{1}_{\mathfrak{h}}\right)\right)\right) \geq \left|\mathrm{tr}_{\mathfrak{h}} \left(A \gamma_\rho\right)\right|^2. \tag{4.19}$$

Proof. We first show *(i)* ⇒ *(ii)*. The properties (4.16)-(4.19) of $\left(\gamma_\rho, \Gamma_\rho\right)$ can be checked by suitable choices of $\mathcal{P}_r$.

a) The first inequality of (4.16) follows by choosing $\mathcal{P}_1 := \sum_{i=1}^M \overline{\alpha}_i c_i$ where $\alpha_i \in \mathbb{C}$ and $M < \infty$:

$$\begin{aligned} 0 \leq \mathrm{tr}_{\mathcal{F}} \left(\rho \, \mathcal{P}_1^* \mathcal{P}_1\right) &= \sum_{i,j=1}^M \alpha_i \overline{\alpha}_j \mathrm{tr}_{\mathcal{F}} \left(\rho \, c_i^* c_j\right) \\ &= \sum_{j=1}^M \sum_{i=1}^M \langle \alpha_j \varphi_j, \gamma_\rho(\alpha_i \varphi_i) \rangle_{\mathfrak{h}} = \langle \phi_M, \gamma_\rho \phi_M \rangle_{\mathfrak{h}} \end{aligned} \tag{4.20}$$

with $\phi_M := \sum_{i=1}^M \alpha_i \varphi_i \in \operatorname{span}\{\varphi_k | \, k \in \mathbb{N}\}$. The second inequality derives from the CAR and $\mathcal{P}_1 := \sum_{i=1}^M \alpha_i c_i^*$:

$$
\begin{aligned}
0 \leq \operatorname{tr}_{\mathcal{F}}\left(\rho \mathcal{P}_1^* \mathcal{P}_1\right) &= \sum_{i,j=1}^M \overline{\alpha}_i \alpha_j \operatorname{tr}_{\mathcal{F}}\left(\rho\, c_i c_j^*\right) \\
&= \sum_{i,j=1}^M \overline{\alpha}_i \alpha_j \operatorname{tr}_{\mathcal{F}}\left(\rho\left(\delta_{ij} - c_j^* c_i\right)\right) \\
&= \sum_{i=1}^M \sum_{j=1}^M \left\langle \alpha_i \varphi_i, (\mathbb{1}_{\mathfrak{h}} - \gamma_\rho)(\alpha_j \varphi_j)\right\rangle_{\mathfrak{h}} \\
&= \left\langle \phi_M, (\mathbb{1}_{\mathfrak{h}} - \gamma_\rho)\phi_M\right\rangle_{\mathfrak{h}} . \qquad (4.21)
\end{aligned}
$$

b) By choosing $\mathcal{P}_2 := \mu + \frac{1}{2}\sum_{k,l=1}^M \alpha_{kl}\left(c_k^* c_l - c_l c_k^*\right)$ with $\mu, \alpha_{kl} \in \mathbb{C}$ and $M < \infty$ and calculating $\operatorname{tr}_{\mathcal{F}}\left(\rho \mathcal{P}_2^* \mathcal{P}_2\right)$, we obtain property (4.19):

$$
\begin{aligned}
0 \leq \operatorname{tr}_{\mathcal{F}}\Bigg(\rho\Bigg(\mu + \frac{1}{2}\sum_{k,l=1}^M \alpha_{kl}(c_k^* c_l - c_l c_k^*)\Bigg)^* \\
\times \Bigg(\mu + \frac{1}{2}\sum_{m,n=1}^M \alpha_{mn}(c_m^* c_n - c_n c_m^*)\Bigg)\Bigg) \\
= \operatorname{tr}_{\mathcal{F}}\Bigg(\rho\Bigg(\frac{1}{2}\sum_{k,l=1}^M \alpha_{kl}(c_k^* c_l - c_l c_k^*)\Bigg)^*\Bigg(\frac{1}{2}\sum_{m,n=1}^M \alpha_{mn}(c_m^* c_n - c_n c_m^*)\Bigg)\Bigg) \\
+ 2\operatorname{Re}\Bigg\{\overline{\mu}\operatorname{tr}_{\mathcal{F}}\Bigg(\frac{1}{2}\rho\sum_{k,l=1}^M \alpha_{kl}(c_k^* c_l - c_l c_k^*)\Bigg)\Bigg\} + |\mu|^2 .
\end{aligned}
$$

Now we expand the brackets and use the CAR to reorder the annihilation and creation operators:

$$
\begin{aligned}
0 \leq \sum_{k,l,m,n=1}^M \overline{\alpha}_{kl}\alpha_{mn}\operatorname{tr}_{\mathcal{F}}\Bigg(\rho\Bigg(- c_l^* c_m^* c_k c_n + \delta_{km} c_l^* c_n - \frac{1}{2}\delta_{kl} c_m^* c_n \\
- \frac{1}{2}\delta_{mn} c_l^* c_k + \frac{1}{4}\delta_{kl}\delta_{mn}\Bigg)\Bigg) \\
+ 2\operatorname{Re}\Bigg\{\overline{\mu}\sum_{k,l=1}^M \alpha_{kl}\operatorname{tr}_{\mathcal{F}}\Bigg(\rho\Bigg(c_k^* c_l - \frac{1}{2}\delta_{kl}\Bigg)\Bigg)\Bigg\} + |\mu|^2 .
\end{aligned}
$$

Bearing $\alpha_{kl} = \langle \varphi_k, A\varphi_l\rangle$ and $\operatorname{tr}_{\mathcal{F}}(\rho) = 1$ in mind, we derive from the definitions of Γ_ρ and γ_ρ that

$$0 \leq \sum_{k,l,m,n=1}^{M} \Big\langle \varphi_k \otimes \varphi_n, \Big(-\Gamma_\rho + \mathbb{1}_\mathfrak{h} \otimes \gamma_\rho - \frac{1}{2}\mathrm{Ex}\,(\gamma_\rho \otimes \mathbb{1}\mathfrak{h}) - \frac{1}{2}\mathrm{Ex}\,(\mathbb{1}_\mathfrak{h} \otimes \gamma_\rho) + \frac{1}{4}\mathrm{Ex}\,(\mathbb{1}_\mathfrak{h} \otimes \mathbb{1}_\mathfrak{h}) \Big) (\varphi_m \otimes \varphi_l) \Big\rangle_{\mathfrak{h}\otimes\mathfrak{h}} \times \langle \varphi_l \otimes \varphi_m, (A^* \otimes A)\,(\varphi_k \otimes \varphi_n) \rangle_{\mathfrak{h}\otimes\mathfrak{h}} + 2\,\mathrm{Re}\left\{ \overline{\mu} \sum_{k,l=1}^{M} \langle \varphi_k, A\varphi_l \rangle_\mathfrak{h} \langle \varphi_l, \gamma_\rho \varphi_k \rangle_\mathfrak{h} - \frac{\overline{\mu}}{2} \sum_{k=1}^{M} \langle \varphi_k, A\varphi_k \rangle_\mathfrak{h} \right\} + |\mu|^2 .$$

We can now perform the summations and arrive at

$$\begin{aligned} 0 &\leq \mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}} \Big(\mathrm{Ex}\,(A^* \otimes A) \Big(-\Gamma_\rho + \mathbb{1}_\mathfrak{h} \otimes \gamma_\rho + \frac{1}{2}\mathrm{Ex}\Big(\frac{1}{2}\mathbb{1}_\mathfrak{h} \otimes \mathbb{1}_\mathfrak{h} - \mathbb{1}_\mathfrak{h} \otimes \gamma_\rho - \gamma_\rho \otimes \mathbb{1}_\mathfrak{h} \Big) \Big) \Big) \\ &\quad + 2\,\mathrm{Re}\left\{ \overline{\mu}\,\mathrm{tr}_\mathfrak{h}\,(A\gamma_\rho) - \frac{\overline{\mu}}{2}\,\mathrm{tr}_\mathfrak{h}\,(A) \right\} + |\mu|^2 \\ &= \mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}} \Big((A^* \otimes A) \Big(\Gamma_\rho + (\mathbb{1}_\mathfrak{h} \otimes \gamma_\rho)\mathrm{Ex} + \frac{1}{4}\mathbb{1}_\mathfrak{h} \otimes \mathbb{1}_\mathfrak{h} - \frac{1}{2}(\mathbb{1}_\mathfrak{h} \otimes \gamma_\rho + \gamma_\rho \otimes \mathbb{1}_\mathfrak{h}) \Big) \Big) \\ &\quad + 2\,\mathrm{Re}\left\{ \overline{\mu}\,\mathrm{tr}_\mathfrak{h}\,(A\gamma_\rho) - \frac{\overline{\mu}}{2}\,\mathrm{tr}_\mathfrak{h}\,(A) \right\} + |\mu|^2 . \end{aligned} \tag{4.22}$$

Defining $s \in \mathbb{C}$ by $\mu =: (s + 1/2)\,\mathrm{tr}_\mathfrak{h}\,(A)$, the inequality can be rewritten as

$$\begin{aligned} 0 &\leq \mathrm{tr}_\mathcal{F} \Big(\rho \Big(\mu + \frac{1}{2} \sum_{k,l=1}^{M} \alpha_{kl} (c_k^* c_l - c_l c_k^*) \Big)^* \times \Big(\mu + \frac{1}{2} \sum_{m,n=1}^{M} \alpha_{mn} (c_m^* c_n - c_n c_m^*) \Big) \Big) \\ &= \mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}} \Big((A^* \otimes A) \Big(\Gamma_\rho + |s|^2\,\mathbb{1}_\mathfrak{h} \otimes \mathbb{1}_\mathfrak{h} + \bar{s}\,\mathbb{1}_\mathfrak{h} \otimes \gamma_\rho + s\,\gamma_\rho \otimes \mathbb{1}_\mathfrak{h} + (\mathbb{1}_\mathfrak{h} \otimes \gamma_\rho)\mathrm{Ex} \Big) \Big). \end{aligned} \tag{4.23}$$

This inequality is valid for all s. We first assume that $\mathrm{tr}_\mathfrak{h}\,(A) = \sum_{i=1}^{M} \alpha_{ii} \neq 0$, then the choice $s := -\frac{\mathrm{tr}_\mathfrak{h}(A\gamma)}{\mathrm{tr}_\mathfrak{h}(A)}$ optimizes the inequality. The conclusion is (4.19):

$$\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\,\big((A^* \otimes A)\,(\Gamma_\rho + \mathrm{Ex}\,(\gamma_\rho \otimes \mathbb{1}_\mathfrak{h})) \big) - \big| \mathrm{tr}_\mathfrak{h}\,(A\gamma_\rho) \big|^2 \geq 0. \tag{4.24}$$

Note that (4.23) and (4.24) are equivalent because (4.24) implies (4.23) by

$$\begin{aligned}
&\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left((A^*\otimes A)\left(\Gamma_\rho + \mathrm{Ex}\left(\gamma_\rho \otimes \mathbb{1}_{\mathfrak{h}}\right)\right)\right) \geq \left|\mathrm{tr}_{\mathfrak{h}}\left(A\gamma_\rho\right)\right|^2 \\
&\qquad \geq -\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left((A^*\otimes A)\left(|s|^2\,\mathbb{1}_{\mathfrak{h}}\otimes\mathbb{1}_{\mathfrak{h}} + \bar{s}\,\mathbb{1}_{\mathfrak{h}}\otimes\gamma_\rho + s\,\gamma_\rho\otimes\mathbb{1}_{\mathfrak{h}}\right)\right).
\end{aligned}$$

Conversely, if $\mathrm{tr}_{\mathfrak{h}}(A) = 0$, the choice $\mu = -\mathrm{tr}_{\mathfrak{h}}(A\gamma)$ in (4.22) leads directly to (4.24).

c) Inserting $\mathcal{P}_2 := \sum_{k,l=1}^{M} \overline{\alpha}_{kl} c_k c_l$ into (4.15), yields Inequality (4.17):

$$\begin{aligned}
0 &\leq \mathrm{tr}_{\mathcal{F}}\left(\rho\left(\sum_{k,l=1}^{M}\overline{\alpha}_{kl}c_kc_l\right)^*\left(\sum_{m,n=1}^{M}\overline{\alpha}_{mn}c_mc_n\right)\right) \\
&= \sum_{k,l,m,n=1}^{M}\alpha_{kl}\overline{\alpha}_{mn}\mathrm{tr}_{\mathcal{F}}\left(\rho\, c_l^* c_k^* c_m c_n\right).
\end{aligned}$$

By the definition of Γ_ρ one finds

$$\begin{aligned}
0 &\leq \sum_{k,l,m,n=1}^{M}\alpha_{kl}\overline{\alpha}_{mn}\left\langle\varphi_m\otimes\varphi_n, \Gamma_\rho(\varphi_k\otimes\varphi_l)\right\rangle_{\mathfrak{h}\otimes\mathfrak{h}} \\
&= \left\langle\Psi_M, \Gamma_\rho\Psi_M\right\rangle_{\mathfrak{h}\otimes\mathfrak{h}}
\end{aligned} \tag{4.25}$$

where $\Psi_M := \sum_{i,j=1}^{M}\alpha_{ij}\left(\varphi_i\otimes\varphi_j\right) \in \mathrm{span}\left\{\varphi_k\otimes\varphi_l \mid k,l\in\mathbb{N}\right\}$.

d) Inequality (4.18) follows from (4.15) by choosing $\mathcal{P}_2 := \sum_{k,l=1}^{M}\alpha_{kl}c_k^*c_l^*$:

$$\begin{aligned}
0 &\leq \mathrm{tr}_{\mathcal{F}}\left(\rho\left(\sum_{k,l=1}^{M}\alpha_{kl}c_k^*c_l^*\right)^*\left(\sum_{m,n=1}^{M}\alpha_{mn}c_m^*c_n^*\right)\right) \\
&= \sum_{k,l,m,n=1}^{M}\overline{\alpha}_{kl}\alpha_{mn}\mathrm{tr}_{\mathcal{F}}\left(\rho\, c_l c_k c_m^* c_n^*\right).
\end{aligned}$$

By normal-ordering using the CAR one establishes the required relationship to Γ_ρ and γ_ρ:

$$\begin{aligned}
0 \leq &\sum_{k,l,m,n=1}^{M}\overline{\alpha}_{kl}\alpha_{mn}\mathrm{tr}_{\mathcal{F}^-}\left\{\rho\left(c_m^*c_n^*c_lc_k - \delta_{ln}c_m^*c_k + \delta_{kn}c_m^*c_l\right.\right. \\
&\qquad\qquad \left.\left. + \delta_{lm}c_n^*c_k - \delta_{km}c_n^*c_l - \delta_{lm}\delta_{kn} + \delta_{km}\delta_{ln}\right)\right\} \\
= &\left\langle\sum_{k,l=1}^{M}\alpha_{kl}(\varphi_l\otimes\varphi_k), \left(\Gamma_\rho + (\mathbb{1}_{\mathfrak{h}\otimes\mathfrak{h}} - \mathrm{Ex})(\mathbb{1}_{\mathfrak{h}}\otimes\mathbb{1}_{\mathfrak{h}}\right.\right. \\
&\qquad\qquad \left.\left. - \gamma_\rho\otimes\mathbb{1}_{\mathfrak{h}} - \mathbb{1}_{\mathfrak{h}}\otimes\gamma_\rho)\right)\left(\sum_{m,n=1}^{M}\alpha_{mn}(\varphi_n\otimes\varphi_m)\right)\right\rangle \\
= &\left\langle\Psi_M, \left(\Gamma_\rho + (\mathbb{1}_{\mathfrak{h}\otimes\mathfrak{h}} - \mathrm{Ex})(\mathbb{1}_{\mathfrak{h}}\otimes\mathbb{1}_{\mathfrak{h}} - \gamma_\rho\otimes\mathbb{1}_{\mathfrak{h}} - \mathbb{1}_{\mathfrak{h}}\otimes\gamma_\rho)\right)\Psi_M\right\rangle.
\end{aligned} \tag{4.26}$$

Next we prove *(ii)* ⇒ *(i)*. Thus, we assume that Inequalities (4.16)-(4.19) hold.

e) A general polynomial of degree $r \leq 1$ is of the form $\mathcal{P}_1 = \sum_{k=1}^{M}(\alpha_k c_k^* + \beta_k c_k) + \mu$ with $\mu, \alpha_k, \beta_k \in \mathbb{C}$. Hence, we have to consider

$$\mathrm{tr}_{\mathcal{F}}\left(\rho\, \mathcal{P}_1^* \mathcal{P}_1\right) = \sum_{k,l=1}^{M} \mathrm{tr}_{\mathcal{F}}\left(\rho\left(\alpha_k c_k^* + \beta_k c_k + \mu\right)^* \left(\alpha_l c_l^* + \beta_l c_l + \mu\right)\right). \tag{4.27}$$

We expand the product on the right hand side of (4.27) and compute the traces taking into account that $\mathrm{tr}_{\mathcal{F}}\left(\rho\, c_i^* c_j^*\right) = \mathrm{tr}_{\mathcal{F}}\left(\rho\, c_i c_j\right) = \mathrm{tr}_{\mathcal{F}}\left(\rho\, c_i^*\right) = \mathrm{tr}_{\mathcal{F}}\left(\rho\, c_i\right) = 0$ for every i, j since ρ preserves the particle number. Therefore only three terms in (4.27) are non-vanishing,

$$\mathrm{tr}_{\mathcal{F}}\left(\rho\, \mathcal{P}_1^* \mathcal{P}_1\right) = \sum_{k,l=1}^{M} \mathrm{tr}_{\mathcal{F}}\left(\rho\left(\left(\alpha_k c_k^*\right)^* \left(\alpha_l c_l^*\right) + \left(\beta_k c_k\right)^* \left(\beta_k c_k\right)\right)\right) + |\mu|^2$$

where we additionally use $\mathrm{tr}_{\mathcal{F}}(\rho) = 1$. The sum over the terms in braces is non-negative due to (4.20) and (4.21). The conclusion is $\mathrm{tr}_{\mathcal{F}}\left(\rho\, \mathcal{P}_1^* \mathcal{P}_1\right) \geq 0$.

f) For $r \leq 2$ we have a general polynomial given by

$$\mathcal{P}_2 = \nu + \sum_{k=1}^{M}\left(\alpha_k c_k^* + \beta_k c_k\right) + \sum_{k,l=1}^{M} \alpha_{kl} c_k^* c_l^* + \sum_{k,l=1}^{M} \beta_{kl} c_k c_l + \sum_{k,l=1}^{M} \kappa_{kl} c_k^* c_l + \sum_{k,l=1}^{M} \eta_{kl} c_k c_l^*$$

where $\nu, \alpha_k, \beta_k, \alpha_{kl}, \beta_{kl}, \kappa_{kl}, \eta_{kl} \in \mathbb{C}$ for all $1 \leq k, l \leq M$. Using the CAR, we rewrite $\mathcal{P}_2$ as

$$\mathcal{P}_2 = \mathcal{P}_1 + \mathcal{P}_{2,\alpha} + \mathcal{P}_{2,\beta} + \mathcal{P}_{2,\eta}$$

where

$$\mathcal{P}_1 := \mu + \sum_{k=1}^{M}\left(\alpha_k c_k^* + \beta_k c_k\right), \qquad \mathcal{P}_{2,\alpha} := \sum_{k,l=1} \alpha_{kl} c_k^* c_k^*,$$

$$\mathcal{P}_{2,\beta} := \sum_{k=1}^{M} \beta_{kl} c_k c_l, \qquad \mathcal{P}_{2,\theta} := \sum_{k,l=1}^{M} \theta_{kl}\left(c_k^* c_l - c_l c_k^*\right),$$

and

$$\mu := \nu + \frac{1}{2}\sum_{k=1}^{M}\left(\kappa_{kk} + \eta_{kk}\right), \quad \theta_{kl} := \frac{1}{2}\left(\kappa_{kl} - \eta_{lk}\right).$$

Then

$$
\begin{aligned}
&\mathrm{tr}_{\mathcal{F}}\left(\rho\,\mathcal{P}_2^*\mathcal{P}_2\right)\\
&\quad= \mathrm{tr}_{\mathcal{F}}\left(\rho\left(\mathcal{P}_1^*+\mathcal{P}_{2,\alpha}^*+\mathcal{P}_{2,\beta}^*+\mathcal{P}_{2,\eta}^*\right)\left(\mathcal{P}_1+\mathcal{P}_{2,\alpha}+\mathcal{P}_{2,\beta}+\mathcal{P}_{2,\theta}\right)\right)\\
&\quad= \mathrm{tr}_{\mathcal{F}}\left(\rho\,\mathcal{P}_1^*\mathcal{P}_1\right)+\mathrm{tr}_{\mathcal{F}}\left(\rho\,\mathcal{P}_{2,\alpha}^*\mathcal{P}_{2,\alpha}\right)+\mathrm{tr}_{\mathcal{F}}\left(\rho\,\mathcal{P}_{2,\beta}^*\mathcal{P}_{2,\beta}\right)\\
&\qquad+\mathrm{tr}_{\mathcal{F}}\left(\rho\,\mathcal{P}_{2,\theta}^*\mathcal{P}_{2,\theta}\right)
\end{aligned}
$$

where we use that $\mathrm{tr}_{\mathcal{F}}\left(\rho\,\mathcal{P}_a^*\mathcal{P}_b\right)=0$ whenever $a\neq b$ since ρ conserves the particle number. Now e) implies $\mathrm{tr}_{\mathcal{F}}\left(\rho\,\mathcal{P}_1^*\mathcal{P}_1\right)\geq 0$, (4.26) yields $\mathrm{tr}_{\mathcal{F}}\left(\rho\,\mathcal{P}_{2,\alpha}^*\mathcal{P}_{2,\alpha}\right)\geq 0$ (see d)), we obtain $\mathrm{tr}_{\mathcal{F}}\left(\rho\,\mathcal{P}_{2,\beta}^*\mathcal{P}_{2,\beta}\right)\geq 0$ from (4.25) (see c)), and $\mathrm{tr}_{\mathcal{F}}\left(\rho\,\mathcal{P}_{2,\theta}^*\mathcal{P}_{2,\theta}\right)\geq 0$ follows from (4.24) (see b)). Hence $\mathrm{tr}_{\mathcal{F}}\left(\rho\,\mathcal{P}_2^*\mathcal{P}_2\right)\geq 0$. □

Lemma 4.4 is the algebraic part of the proof of Theorem 4.3. In order to conclude we have to extend the proof to infinite dimensions.

Proof of Theorem 4.3. Since *(ii)* contains (4.16)-(4.19) of Lemma 4.4, the implication *(ii)* ⇒ *(i)* is obvious. For *(i)* ⇒ *(ii)* let ϕ,ψ and Φ,Ψ be normalized vectors in $\mathfrak{h}$ and $\mathfrak{h}\otimes\mathfrak{h}$, respectively, and set $\alpha_i:=\langle\varphi_i,\phi\rangle_{\mathfrak{h}}$, $\beta_i:=\langle\varphi_i,\psi\rangle_{\mathfrak{h}}$, and $\alpha_{ij}:=\langle\varphi_i\otimes\varphi_j,\Phi\rangle_{\mathfrak{h}\otimes\mathfrak{h}}$, $\beta_{ij}:=\langle\varphi_i\otimes\varphi_j,\Psi\rangle_{\mathfrak{h}\otimes\mathfrak{h}}$ for all $i,j\in\mathbb{N}$. For $M\in\mathbb{N}$ we define the orthogonal projection $P_M:=\sum_{k=1}^M|\varphi_k\rangle\langle\varphi_k|$ and set $\phi_M:=P_M\phi=\sum_{i=1}^M\alpha_i\varphi_i$ and $\Psi_M:=(P_M\otimes P_M)\Psi=\sum_{i,j=1}^M\beta_{ij}\left(\varphi_i\otimes\varphi_j\right)$. The admissibility and the G-, P-, and Q-conditions follow from Lemma 4.4 as follows:

a) For the 1-pdm we have $\|\gamma_\rho\|_{\mathrm{op}}<\infty$ since

$$
\left|\langle\phi,\gamma_\rho\psi\rangle_{\mathfrak{h}}\right|=\left|\mathrm{tr}_{\mathcal{F}}\left(\rho\,c^*(\psi)c(\phi)\right)\right|\leq\mathrm{tr}_{\mathcal{F}}\left(|\rho|\right)\|\psi\|\|\phi\|=\mathrm{tr}_{\mathcal{F}}\left(|\rho|\right)<\infty
$$

by the Cauchy–Schwarz inequality and $c^*(\phi)c(\phi)\leq\mathbb{1}_{\mathcal{F}}\langle\phi,\phi\rangle_{\mathfrak{h}}$. Afterwards we infer by the triangle inequality

$$
\begin{aligned}
\left|\langle\phi,\gamma_\rho\phi\rangle_{\mathfrak{h}}-\langle\phi_M,\gamma_\rho\phi_M\rangle_{\mathfrak{h}}\right| &= \left|\langle\phi-\phi_M,\gamma_\rho\phi\rangle_{\mathfrak{h}}+\langle\phi_M,\gamma_\rho(\phi-\phi_M)\rangle_{\mathfrak{h}}\right|\\
&\leq\left|\langle\phi-\phi_M,\gamma_\rho\phi\rangle_{\mathfrak{h}}\right|+\left|\langle\phi_M,\gamma_\rho(\phi-\phi_M)\rangle_{\mathfrak{h}}\right|\\
&\leq\|\phi-\phi_M\|\left(\|\phi\|+\|\phi_M\|\right)\|\gamma_\rho\|_{\mathrm{op}}\\
&\leq 2\,\|\phi-\phi_M\|\|\gamma_\rho\|_{\mathrm{op}}. \qquad (4.28)
\end{aligned}
$$

As $M\to\infty$, $\|\phi-\phi_M\|$ vanishes. With $\langle\phi_M,\gamma_\rho\phi_M\rangle_{\mathfrak{h}}\geq 0$ we conclude that also $\langle\phi,\gamma_\rho\phi\rangle_{\mathfrak{h}}\geq 0$ for all $\phi\in\mathfrak{h}$. The same argument with γ_ρ replaced by $\mathbb{1}_{\mathfrak{h}}-\gamma_\rho$ leads to $\langle\phi,(\mathbb{1}_{\mathfrak{h}}-\gamma_\rho)\phi\rangle_{\mathfrak{h}}\geq 0$ for all $\phi\in\mathfrak{h}$.

b) $\gamma_\rho \in \mathcal{L}^1(\mathfrak{h})$ follows by monotone convergence since $\gamma_\rho \geq 0$. For any ONB $\{\psi_i\}_{i=1}^\infty$ of $\mathfrak{h}$ and $\epsilon > 0$ we have

$$\begin{aligned}
&\sum_{k=1}^{\infty} \langle \psi_k, \gamma_\rho \psi_k \rangle_{\mathfrak{h}} \\
&\quad \leq \sup_M \left\{ \mathrm{tr}_{\mathcal{F}} \left(\rho \sum_{k=1}^{M} c_k^* c_k \right) \right\} \\
&\quad = (N+\epsilon) \sup_M \left\{ \mathrm{tr}_{\mathcal{F}} \left(\rho \left(\frac{1}{\widehat{\mathbb{N}}+\epsilon} \right)^{\frac{1}{2}} \left(\sum_{k=1}^{M} c_k^* c_k \right) \left(\frac{1}{\widehat{\mathbb{N}}+\epsilon} \right)^{\frac{1}{2}} \right) \right\} \\
&\quad \leq (N+\epsilon)\, \mathrm{tr}_{\mathcal{F}} (|\rho|) < \infty
\end{aligned}$$

since $\widehat{\mathbb{N}}\rho = N\rho$ and $\left\| \left(\frac{1}{\widehat{\mathbb{N}}+\epsilon} \right)^{\frac{1}{2}} \left(\sum_{k=1}^{M} c_k^* c_k \right) \left(\frac{1}{\widehat{\mathbb{N}}+\epsilon} \right)^{\frac{1}{2}} \right\|_{\mathrm{op}} \leq 1.$

c) Due to b) we can compute $\sum_{k=1}^\infty \langle \varphi_k, \gamma_\rho \varphi_k \rangle_{\mathfrak{h}}$ using monotone convergence and $\widehat{\mathbb{N}}\rho = N\rho$. This gives the trace of γ_ρ.

$$\begin{aligned}
\mathrm{tr}_{\mathfrak{h}} (\gamma_\rho) := \sum_{k=1}^{\infty} \langle \varphi_k, \gamma_\rho \varphi_k \rangle_{\mathfrak{h}} &= \sum_{k=1}^{\infty} \mathrm{tr}_{\mathcal{F}} (\rho\, c_k^* c_k) \\
&= \mathrm{tr}_{\mathcal{F}} \left(\rho \sum_{k=1}^{\infty} c_k^* c_k \right) = \mathrm{tr}_{\mathcal{F}} \left(\rho \widehat{\mathbb{N}} \right) = N.
\end{aligned}$$

d) For any basis of $\mathfrak{h}$ the identities $\mathrm{Ex}\,\Gamma_\rho = \Gamma_\rho\,\mathrm{Ex} = -\Gamma_\rho$ are a consequence of the definition of Γ_ρ and the CAR.

e) We conclude from the definition of Γ_ρ by the Cauchy–Schwarz inequality that

$$\begin{aligned}
\left| \langle \Psi, \Gamma_\rho \Phi \rangle_{\mathfrak{h}\otimes\mathfrak{h}} \right| &= \left| \mathrm{tr}_{\mathcal{F}} \left(\rho \left(\sum_{m,n=1}^{\infty} \beta_{mn} c_n c_m \right)^* \left(\sum_{k,l=1}^{\infty} \alpha_{kl} c_l c_k \right) \right) \right| \\
&\leq \mathrm{tr}_{\mathcal{F}} (|\rho|) \, \|\Psi\| \|\Phi\| = \mathrm{tr}_{\mathcal{F}} (|\rho|) < \infty.
\end{aligned}$$

Therefore, we have $\|\Gamma_\rho\|_{\mathrm{op}} < \infty$. Afterwards we infer analogously to (4.28)

$$\left| \langle \Psi, \Gamma_\rho \Psi \rangle_{\mathfrak{h}\otimes\mathfrak{h}} - \langle \Psi_M, \Gamma_\rho \Psi_M \rangle_{\mathfrak{h}\otimes\mathfrak{h}} \right| \leq 2 \|\Psi - \Psi_M\| \|\Gamma_\rho\|_{\mathrm{op}}$$

which tends to zero as $M \to \infty$ due to the definition of Ψ_M. With $\langle \Psi_M | \Gamma_\rho \Psi_M \rangle_{\mathfrak{h}\otimes\mathfrak{h}} \geq 0$ from (4.25) this implies $\langle \Psi | \Gamma_\rho \Psi \rangle_{\mathfrak{h}\otimes\mathfrak{h}} \geq 0$ for all $\Psi \in \mathfrak{h} \otimes \mathfrak{h}$.

f) In order to prove that $\Gamma_\rho \in \mathcal{L}^1(\mathfrak{h}\otimes\mathfrak{h})$, we show that there is an ONB $\{\psi_i\}_{i=1}^\infty$ of $\mathfrak{h}$ such that $\sum_{k,l=1}^\infty \langle \psi_k \otimes \psi_l, \Gamma_\rho(\psi_k \otimes \psi_l) \rangle_{\mathfrak{h}\otimes\mathfrak{h}}$ is finite, again using $\Gamma_\rho \geq 0$. For any $\epsilon > 0$, we have using $\widehat{\mathbb{N}}\rho = N\rho$ and monotone convergence

$$\sum_{k,l=1}^{\infty} \langle \psi_k \otimes \psi_l, \Gamma_\rho(\psi_k \otimes \psi_l) \rangle_{\mathfrak{h}\otimes\mathfrak{h}} \leq \sup_M \left\{ \sum_{k,l=1}^{M} \mathrm{tr}_{\mathcal{F}} \left(\rho\, c_l^* c_k c_k^* c_l \right) \right\}$$
$$= \sup_M \left\{ \mathrm{tr}_{\mathcal{F}} \left(\rho \left[\left(\sum_{k=1}^{M} c_k^* c_k \right)^2 - \left(\sum_{k=1}^{M} c_k^* c_k \right) \right] \right) \right\}$$
$$\leq \sup_M \left\{ \left(N^2 + \epsilon \right) \times \mathrm{tr}_{\mathcal{F}} \left(|\rho| \left(\frac{1}{\widehat{\mathbb{N}}^2 + \epsilon} \right)^{\frac{1}{2}} \left(\sum_{k=1}^{M} c_k^* c_k \right)^2 \left(\frac{1}{\widehat{\mathbb{N}}^2 + \epsilon} \right)^{\frac{1}{2}} \right) \right\}$$
$$\leq \left(N^2 + \epsilon \right) \mathrm{tr}_{\mathcal{F}} \left(|\rho| \right) < \infty$$

since $\sum_{k=1}^{M} c_k^* c_k \geq 0$ and due to $\left(\sum_{k=1}^{M} c_k^* c_k \right)^2 \leq \widehat{\mathbb{N}}^2$

$$\left\| \left(\frac{1}{\widehat{\mathbb{N}}^2 + \epsilon} \right)^{\frac{1}{2}} \left(\sum_{k=1}^{M} c_k^* c_k \right)^2 \left(\frac{1}{\widehat{\mathbb{N}}^2 + \epsilon} \right)^{\frac{1}{2}} \right\|_{\mathrm{op}} \leq 1.$$

g) In order to check (4.24) for any bounded A (not necessarily of finite rank) we abbreviate $\Lambda_{\mathrm{G}} := \Gamma_\rho + \mathrm{Ex}\left(\gamma_\rho \otimes \mathbb{1}_{\mathfrak{h}} \right) - \gamma_\rho \otimes \gamma_\rho$ and set $A_M := P_M A P_M$. Clearly A_M is of finite rank and we observe

$$\begin{aligned} &\left| \mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}} \left((A^* \otimes A) \Lambda_{\mathrm{G}} \right) - \mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}} \left((A_M^* \otimes A_M) \Lambda_{\mathrm{G}} \right) \right| \\ &\quad = \left| \mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}} \left(\left[(A - A_M)^* \otimes A + A_M^* \otimes (A - A_M) \right] \Lambda_{\mathrm{G}} \right) \right| \\ &\quad = \left| \mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}} \left(\left[\left(P_M A^* P_M^\perp + P_M^\perp A^* P_M + P_M^\perp A^* P_M^\perp \right) \otimes A \right. \right. \right. \\ &\qquad\qquad \left. \left. \left. + A_M^* \otimes \left(P_M^\perp A P_M + P_M A P_M^\perp + P_M^\perp A P_M^\perp \right) \right] \Lambda_{\mathrm{G}} \right) \right| \end{aligned} \tag{4.29}$$

using $P_M^\perp := \mathbb{1}_{\mathfrak{h}} - P_M$. For $\left| \mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}} \left((P_M^\perp A^* P_M \otimes A) \Lambda_{\mathrm{G}} \right) \right|$, for instance, we find

$$\begin{aligned} &\left| \mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}} \left(\left(P_M^\perp A^* P_M \otimes A \right) \Lambda_{\mathrm{G}} \right) \right| \\ &\quad = \left| \mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}} \left(\left(P_M^\perp A^* P_M \otimes A \right) \Gamma_\rho \right) + \mathrm{tr}_{\mathfrak{h}} \left(P_M^\perp A^* P_M \gamma_\rho A \right) \right. \\ &\qquad\qquad \left. - \mathrm{tr}_{\mathfrak{h}} \left(P_M^\perp A^* P_M \gamma_\rho \right) \mathrm{tr}_{\mathfrak{h}} \left(A \gamma_\rho \right) \right| \\ &\quad \leq \left| \mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}} \left(\left(P_M^\perp A^* P_M \otimes A \right) \Gamma_\rho \right) \right| + \left| \mathrm{tr}_{\mathfrak{h}} \left(P_M^\perp A^* P_M \gamma_\rho A \right) \right| \\ &\qquad + \left| \mathrm{tr}_{\mathfrak{h}} \left(P_M^\perp A^* P_M \gamma_\rho \right) \mathrm{tr}_{\mathfrak{h}} \left(A \gamma_\rho \right) \right|. \end{aligned}$$

Since $\Gamma_\rho \geq 0$ due to the P-condition (see e)), $P_M^\perp, P_M \geq 0$, and $\widehat{\mathbb{N}}\rho = N\rho$, we have, on the one hand,

$$\begin{aligned} \left| \mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}} \left(\left(P_M^\perp A^* P_M \otimes A \right) \Gamma_\rho \right) \right| &\leq \|A\|_{\mathrm{op}}^2 \, \mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}} \left(\left(P_M^\perp \otimes \mathbb{1}_{\mathfrak{h}} \right) \Gamma_\rho \right) \\ &= (N-1) \, \|A\|_{\mathrm{op}}^2 \, \mathrm{tr}_{\mathfrak{h}} \left(P_M^\perp \gamma_\rho \right), \end{aligned}$$

and, on the other hand, with $0 \leq \gamma_\rho \leq \mathbb{1}_\mathfrak{h}$ and $P_M \leq \mathbb{1}_\mathfrak{h}$

$$\left|\mathrm{tr}_\mathfrak{h}\left(P_M^\perp A^* P_M \gamma_\rho A\right)\right| \leq \|A\|_{\mathrm{op}}^2 \,\mathrm{tr}_\mathfrak{h}\left(P_M^\perp \gamma_\rho\right)$$

and

$$\left|\mathrm{tr}_\mathfrak{h}\left(P_M^\perp A^* P_M \gamma_\rho\right) \mathrm{tr}_\mathfrak{h}\left(A\gamma_\rho\right)\right| \leq N \|A\|_{\mathrm{op}}^2 \,\mathrm{tr}_\mathfrak{h}\left(P_M^\perp \gamma_\rho\right).$$

Note that $\mathrm{tr}_\mathfrak{h}\left(P_M^\perp \gamma_\rho\right) = \sum_{k=M+1}^\infty \langle \varphi_k, \gamma_\rho \varphi_k\rangle_\mathfrak{h} \to 0$ as $M \to \infty$ since $\sum_{k=1}^\infty \langle \varphi_k, \gamma_\rho \varphi_k\rangle = \mathrm{tr}_\mathfrak{h}\left(\gamma_\rho\right) = N$ is convergent. Analogously one finds that all terms on the right hand side of (4.29) tend to zero as $M \to \infty$. This in turn implies $\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(A^* \otimes A\right)\Lambda_\mathrm{G}\right) \geq 0$ for any bounded A since $\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(A_M^* \otimes A_M\right)\Lambda_\mathrm{G}\right) \geq 0$ due to (4.24).

h) Again by the Cauchy–Schwarz inequality we find

$$\begin{aligned}
&\left|\left\langle \Psi, \left(\Gamma_\rho + (\mathbb{1}_{\mathfrak{h}\otimes\mathfrak{h}} - \mathrm{Ex})(\mathbb{1}_\mathfrak{h} \otimes \mathbb{1}_\mathfrak{h} - \gamma_\rho \otimes \mathbb{1}_\mathfrak{h} - \mathbb{1}_\mathfrak{h} \otimes \gamma_\rho)\right)\Phi\right\rangle_{\mathfrak{h}\otimes\mathfrak{h}}\right| \\
&\quad = \left|\mathrm{tr}_{\mathcal{F}^-}\left\{\rho\left(\sum_{m,n=1}^\infty \overline{\beta}_{mn} c_m c_n\right)\left(\sum_{k,l=1}^\infty \overline{\alpha}_{kl} c_k c_l\right)^*\right\}\right| \\
&\quad \leq \mathrm{tr}_\mathcal{F}\left(|\rho|\right) \|\Psi\| \|\Phi\|
\end{aligned}$$

and, therefore, $\|\Gamma_\rho + (\mathbb{1}_{\mathfrak{h}\otimes\mathfrak{h}} - \mathrm{Ex})(\mathbb{1}_\mathfrak{h} \otimes \mathbb{1}_\mathfrak{h} - \gamma_\rho \otimes \mathbb{1}_\mathfrak{h} - \mathbb{1}_\mathfrak{h} \otimes \gamma_\rho)\|_{\mathrm{op}} < \infty$. Following (4.28) with $\Gamma_\rho + (\mathbb{1}_{\mathfrak{h}\otimes\mathfrak{h}} - \mathrm{Ex})(\mathbb{1}_\mathfrak{h} \otimes \mathbb{1}_\mathfrak{h} - \gamma_\rho \otimes \mathbb{1}_\mathfrak{h} - \mathbb{1}_\mathfrak{h} \otimes \gamma_\rho)$ instead of Γ_ρ, we arrive at

$$\left\langle \Psi, \left(\Gamma_\rho + (\mathbb{1}_{\mathfrak{h}\otimes\mathfrak{h}} - \mathrm{Ex})(\mathbb{1}_\mathfrak{h} \otimes \mathbb{1}_\mathfrak{h} - \gamma_\rho \otimes \mathbb{1}_\mathfrak{h} - \mathbb{1}_\mathfrak{h} \otimes \gamma_\rho)\right)\Psi\right\rangle_{\mathfrak{h}\otimes\mathfrak{h}} \geq 0$$

for all $\Psi \in \mathfrak{h} \otimes \mathfrak{h}$.

$\left(\gamma_\rho, \Gamma_\rho\right)$ obeys the P-, G-, and Q-conditions by e), g) and h). The admissibility is ensured in a) to d), and f). □

A simple consequence of Theorem 4.3 is

Corollary 4.5. *Let $N \in \mathbb{N}$ and assume that (γ, Γ) is N-representable. Then (γ, Γ) is admissible and fulfills the G-, P-, and Q-conditions.*

Proof. Since (γ, Γ) is N-representable, there exists a density matrix $\rho \in \mathcal{L}_+^1(\mathcal{F}^-)$ with $(\gamma, \Gamma) \equiv \left(\gamma_\rho, \Gamma_\rho\right)$. By the last theorem (γ, Γ) then is admissible and fulfills the G-, P-, and Q-conditions. □

Remark 4.6. The G-condition (4.19) seems to be asymmetric in terms of γ_ρ. However, since $\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(A \otimes B\right)\Gamma_\rho\right) = \mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(B \otimes A\right)\Gamma_\rho\right)$, it is easy to show that also $\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(A^* \otimes A\right)\left(\Gamma_\rho + \mathrm{Ex}\left(\mathbb{1}_\mathfrak{h} \otimes \gamma_\rho\right)\right)\right) \geq \left|\mathrm{tr}_\mathfrak{h}\left(A\gamma_\rho\right)\right|^2$ holds. Thus, we have a symmetrized, but weaker, G-condition given by

$$\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(A^* \otimes A\right)\left(\Gamma_\rho + \frac{1}{2}\mathrm{Ex}\left(\mathbb{1}_\mathfrak{h} \otimes \gamma_\rho + \gamma_\rho \otimes \mathbb{1}_\mathfrak{h}\right)\right)\right) \geq \left|\mathrm{tr}_\mathfrak{h}\left(A\gamma_\rho\right)\right|^2.$$

4 Correlation Inequalities from G- and P-Conditions

In [Bac92] a lower bound on the difference of the ground state functional $\mathcal{E}(\gamma,\Gamma)$ and the Hartree–Fock functional $\mathcal{E}(\gamma,(\mathbb{1}_{\mathfrak{h}\otimes\mathfrak{h}}-\mathrm{Ex}(\gamma\otimes\gamma)))$, i.e.,

$$\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(V\Gamma^{(\mathrm{T})}\right)=\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(V\left(\Gamma-\left(\mathbb{1}_{\mathfrak{h}\otimes\mathfrak{h}}-\mathrm{Ex}\right)(\gamma\otimes\gamma)\right)\right), \tag{4.30}$$

is derived using the decomposition of the potential V according to Fefferman and de la Llave [FdlL86]. It turns out that this decomposition is also useful to derive lower bounds only by means of N-representability. The main result of this section is the following theorem.

Theorem 4.7 (Fermion Correlation Inequality). *Let $X=X^*=X^2\in\mathcal{B}(\mathfrak{h})$ be an orthogonal projection on $\mathfrak{h}$. Assume that (γ,Γ) is admissible and fulfills the G- and P-conditions. Then*

$$\begin{aligned}&\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left((X\otimes X)\,\Gamma^{(\mathrm{T})}\right)\\&\quad\geq-\mathrm{tr}_{\mathfrak{h}}(X\gamma)\min\Big\{1;\;38\,\mathrm{tr}_{\mathfrak{h}}\left(X\left(\gamma-\gamma^2\right)\right)\\&\qquad\qquad+4\Big[\mathrm{tr}_{\mathfrak{h}}\left(X\left(\gamma-\gamma^2\right)\right)\left(2+8\,\mathrm{tr}_{\mathfrak{h}}\left(X\left(\gamma-\gamma^2\right)\right)^2\right)\Big]^{\frac{1}{2}}\Big\}.\end{aligned} \tag{4.31}$$

Proof. The proof is carried out in several parts in the following subsections. The first inequality is derived in Theorem 4.10. The second inequality follows from Theorems 4.21, 4.23 and 4.25. □

In order to apply Theorem 4.7 to $\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(V\Gamma^{(\mathrm{T})}\right)$ the potential V on $\mathfrak{h}\otimes\mathfrak{h}$ is decomposed into an integral of a tensor product of two copies of the one-particle operator X. This decomposition is called Fefferman–de la Llave identity.

Lemma 4.8 (Fefferman–de la Llave Identity). *For all $x,y\in\mathbb{R}^3$, $x\neq y$ the identity*

$$\frac{1}{|x-y|}=\int_0^\infty\frac{\mathrm{d}r}{\pi r^5}\int_{\mathbb{R}^3}\mathrm{d}^3z\,\chi_{B(z,r)}(x)\,\chi_{B(z,r)}(y) \tag{4.32}$$

holds true where $\chi_{B(z,r)}$ is the characteristic function of the ball of radius $r>0$ centered at $z\in\mathbb{R}^3$, $B(z,r):=\left\{x\in\mathbb{R}^3\mid|x-z|\leq r\right\}$.

The proof of the decomposition can be found in the original work of Fefferman and de la Llave in [FdlL86]. In [HS02] Hainzl and Seiringer have derived sufficient conditions on a pair potential $V:\mathbb{R}^n\to\mathbb{R}$ such that it admits a decomposition of the form (4.32).

Remark 4.9. The multiplication operator corresponding to $\chi_{B(z,r)}$ is denoted by $X_{r,z}\equiv X$. Clearly

$$X=X^*=X^2\in\mathcal{B}(\mathfrak{h}) \tag{4.33}$$

is an orthogonal projection.

Instead of $\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(V\Gamma^{(\mathrm{T})}\right)$ we consider from now on

$$\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left((X\otimes X)\,\Gamma^{(\mathrm{T})}\right) = \mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left((X\otimes X)\left(\Gamma - (\mathbb{1}_{\mathfrak{h}\otimes\mathfrak{h}} - \mathrm{Ex})\,(\gamma\otimes\gamma)\right)\right). \tag{4.34}$$

A first estimation of this quantity is immediately obtained by applying the G-condition directly on $\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left((X\otimes X)\,\Gamma\right)$. This yields the first inequality of (4.31).

Theorem 4.10. *Let $X \in \mathcal{B}(\mathfrak{h})$ be an orthogonal projection. Assume that (γ, Γ) is admissible and fulfills the G-condition. Then*

$$\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left((X\otimes X)\,\Gamma^{(\mathrm{T})}\right) \geq -\,\mathrm{tr}_{\mathfrak{h}}\left(X\gamma\right).$$

Proof. As mentioned we apply the G-condition (4.14) with $A^* = A := X$ directly on $\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left((X\otimes X)\,\Gamma\right)$. Carrying out the trace the Hartree–Fock part while estimating the part with the 2-pdm by the G-condition, we obtain

$$\begin{aligned}
&\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left((X\otimes X)\left(\Gamma - (\mathbb{1}_{\mathfrak{h}\otimes\mathfrak{h}} - \mathrm{Ex})\,(\gamma\otimes\gamma)\right)\right)\\
&\quad\geq \left(\mathrm{tr}_{\mathfrak{h}}\left(X\gamma\right)\right)^2 - \mathrm{tr}_{\mathfrak{h}}\left(X\gamma\right) - \left(\mathrm{tr}_{\mathfrak{h}}\left(X\gamma\right)\right)^2 + \mathrm{tr}_{\mathfrak{h}}\left(X\gamma X\gamma\right)\\
&\quad\geq -\,\mathrm{tr}_{\mathfrak{h}}\left(X\gamma\right).
\end{aligned} \tag{4.35}$$

The last inequality follows from $\mathrm{tr}_{\mathfrak{h}}\left(X\gamma X\gamma\right) = \mathrm{tr}_{\mathfrak{h}}\left(X\gamma X\gamma X\right) \geq 0$. □

The goal of the next subsections is an estimation of $\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left((X\otimes X)\,\Gamma\right)$ in terms of $\mathrm{tr}_{\mathfrak{h}}\left(X\left(\gamma - \gamma^2\right)\right)$.

4.1 Preparation

A crucial step in [Bac92] is the decomposition of the spectrum of γ into eigenvalues which are larger than $1/2$ and those which are smaller or equal $1/2$. Following this step, the decomposition is denoted by two orthogonal projections, P and $P^\perp$ (a comparable strategy was also used by Graf and Solovej in [GS94]). The first one, P, projects on the space which is spanned by the eigenvectors of γ corresponding to eigenvalues larger than $1/2$. The second one treats the eigenvectors with eigenvalues smaller or equal $1/2$. Furthermore, the eigenvectors of γ, $\{\varphi_i \,|\, \gamma\varphi_i = \lambda_i\varphi_i\}_{i=1}^{\infty}$, are used as an ONB of $\mathfrak{h}$ which we mainly refer to. In this basis the two projections can be defined straightforwardly.

Definition 4.11. On $\mathfrak{h}$ the orthogonal projections P and $P^\perp$ are defined by

$$P := \mathbb{1}\left[\gamma > \frac{1}{2}\right] = \sum_{k>\frac{1}{2}} |\varphi_k\rangle\,\langle\varphi_k| \text{ and } P^\perp := \mathbb{1}\left[\gamma \leq \frac{1}{2}\right] = \sum_{k\leq\frac{1}{2}} |\varphi_k\rangle\,\langle\varphi_k|. \tag{4.36}$$

Here the summation over "$k > 1/2$" denotes the summation over indices $\left\{k \,\middle|\, \lambda_k > \frac{1}{2}\right\}$ and for "$k \leq \frac{1}{2}$" analogously. Obviously

$$P + P^\perp = \mathbb{1}_{\mathfrak{h}}, \quad PP^\perp = P^\perp P = 0, \quad P\gamma = \gamma P \quad \text{and} \quad P^\perp\gamma = \gamma P^\perp.$$

Moreover, the projections are bounded above:

Lemma 4.12. *For P and $P^\perp$ defined in (4.36) the inequalities*

$$P \le 2\gamma \quad \textit{and} \quad P^\perp \le 2\left(\mathbb{1}_{\mathfrak{h}} - \gamma\right) \tag{4.37}$$

hold true.

Note that since $\mathrm{rk}\,\{P\} \le 2N$, P is of finite rank and hence trace class.

Proof. Using the definition of the projections together with $0 \le \gamma \le \mathbb{1}_{\mathfrak{h}}$, we find for P:

$$P = \sum_{k>\frac{1}{2}} |\varphi_k\rangle\langle\varphi_k| \le \sum_{k>\frac{1}{2}} 2\lambda_k |\varphi_k\rangle\langle\varphi_k| \le 2\sum_{k=1}^{\infty} \lambda_k |\varphi_k\rangle\langle\varphi_k| = 2\gamma,$$

and for $P^\perp$:

$$P^\perp = \sum_{k\le\frac{1}{2}} |\varphi_k\rangle\langle\varphi_k| \le \sum_{k\le\frac{1}{2}} 2\left(1-\lambda_k\right) |\varphi_k\rangle\langle\varphi_k| \le 2\left(\mathbb{1}_{\mathfrak{h}} - \gamma\right). \qquad \square$$

Because $P^\perp + P = \mathbb{1}_{\mathfrak{h}}$, we can expand $\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left((X\otimes X)\,\Gamma\right)$ into three parts to have expressions on which we can apply the conditions on (γ, Γ). We call these three parts Main Part (MP), Remainder (R), and Main Error Term (MET).

Lemma 4.13. *Let $X \in \mathcal{B}(\mathfrak{h})$ be an orthogonal projection, P and $P^\perp$ as in Definition 4.11. Then*

$$\begin{aligned}
&\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left((X\otimes X)\,\Gamma\right) \\
&\quad = \mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left((PXP\otimes PXP)\,\Gamma\right) + 4\,\mathrm{Re}\left\{\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(PXP\otimes P^\perp XP\right)\Gamma\right)\right\} \\
&\qquad\qquad + 2\,\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(PXP^\perp\otimes P^\perp XP\right)\Gamma\right) \\
&\qquad + \mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(P^\perp XP^\perp\otimes P^\perp XP^\perp\right)\Gamma\right) + 2\,\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(P^\perp XP^\perp\otimes PXP\right)\Gamma\right) \\
&\qquad\qquad + 4\,\mathrm{Re}\left\{\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(P^\perp XP\otimes P^\perp XP^\perp\right)\Gamma\right)\right\} \\
&\qquad + 2\,\mathrm{Re}\left\{\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(PXP^\perp\otimes PXP^\perp\right)\Gamma\right)\right\}.
\end{aligned} \tag{4.38}$$

Proof. After replacing the identity operator on each side of X in each factor of the tensor product $X\otimes X$ by $\left(P+P^\perp\right)$, we expand the r.h.s. of

$$\begin{aligned}
&\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left((X\otimes X)\,\Gamma\right) \\
&\quad = \mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(\left(P+P^\perp\right)X\left(P+P^\perp\right)\otimes\left(P+P^\perp\right)X\left(P+P^\perp\right)\right)\Gamma\right).
\end{aligned}$$

Using $\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left((A\otimes B)\,\Gamma\right) = \mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left((B\otimes A)\,\Gamma\right)$ as a consequence of $\mathrm{Ex}\,\Gamma\,\mathrm{Ex} = \Gamma$, we arrive at the assertion after rearranging. $\square$

Afterwards we collect the terms of the r.h.s. of Equation (4.38) in a suitable way. Note that compared to [Bac92] the definitions of the Main Part and the Remainder are slightly changed.

Definition 4.14. The term

$$T_{\mathrm{MP}} := \mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left((PXP\otimes PXP)\,\Gamma\right) + 4\ \mathrm{Re}\left\{\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(PXP\otimes P^{\perp}XP\right)\Gamma\right)\right\} + 4\,\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(PXP^{\perp}\otimes P^{\perp}XP\right)\Gamma\right)$$

is called Main Part,

$$\begin{aligned} T_{\mathrm{R}} := {} & \mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(P^{\perp}XP^{\perp}\otimes P^{\perp}XP^{\perp}\right)\Gamma\right) \\ & + 4\ \mathrm{Re}\left\{\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(P^{\perp}XP\otimes P^{\perp}XP^{\perp}\right)\Gamma\right)\right\} \\ & + 2\,\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(P^{\perp}XP^{\perp}\otimes PXP\right)\Gamma\right) + 2\,\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(PXP^{\perp}\otimes P^{\perp}XP\right)\Gamma\right) \end{aligned}$$

is called Remainder, and

$$T_{\mathrm{MET}} := 2\ \mathrm{Re}\left\{\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(PXP^{\perp}\otimes PXP^{\perp}\right)\Gamma\right)\right\}$$

is called Main Error Term.

One estimate is used more than once when considering the terms in the Remainder and Main Error Term. This estimate requires the following lemma.

Lemma 4.15. *Let $\{\psi_i\}_{i=1}^{\infty}$ be an ONB of $\mathfrak{h}$ and $Q = Q^* = Q^2$, $Q^{\perp} := \mathbb{1}_{\mathfrak{h}} - Q$, and $Y = Y^* = Y^2 \in \mathcal{B}(\mathfrak{h})$ orthogonal projections. For $r, s \in \mathbb{N}$ we define*

$$B(r,s) := |QY\psi_r\rangle\left\langle Q^{\perp}Y\psi_s\right| \in \mathcal{B}(\mathfrak{h}).$$

Then we have

$$\sum_{r,s=1}^{\infty}\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left((B^*(r,s)\otimes B(r,s))\left(\Gamma + \mathrm{Ex}\left(\gamma\otimes\mathbb{1}_{\mathfrak{h}}\right)\right)\right) = \mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(QYQ\otimes Q^{\perp}YQ^{\perp}\right)\left(-\Gamma + \mathbb{1}_{\mathfrak{h}}\otimes\gamma\right)\right). \tag{4.39}$$

Proof. Denoting $K := \sum_{r,s=1}^{\infty}\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left((B^*(r,s)\otimes B(r,s))\left(\Gamma + \mathrm{Ex}\left(\gamma\otimes\mathbb{1}_{\mathfrak{h}}\right)\right)\right)$, we calculate the trace using the ONB $\{\psi_i\}_{i=1}^{\infty}$ of $\mathfrak{h}$.

$$K = \sum_{r,s=1}^{\infty}\sum_{k,l,m,n=1}^{\infty}\langle\psi_k\otimes\psi_l, (B^*(r,s)\otimes B(r,s))(\psi_m\otimes\psi_n)\rangle_{\mathfrak{h}\otimes\mathfrak{h}} \times\langle\psi_m\otimes\psi_n, \left(\Gamma + \mathrm{Ex}\left(\gamma\otimes\mathbb{1}_{\mathfrak{h}}\right)\right)(\psi_k\otimes\psi_l)\rangle_{\mathfrak{h}\otimes\mathfrak{h}}.$$

In the next step the definition of $B(r,s)$ together with the notation of matrix elements by $(A)_{ij} := \langle\psi_i, A\psi_j\rangle_{\mathfrak{h}}$ for any $A \in \mathcal{B}(\mathfrak{h})$ can be used to write

$$K = \sum_{r,s=1}^{\infty}\sum_{k,l,m,n=1}^{\infty}(YQ)_{rm}\left(Q^{\perp}Y\right)_{ks}(QY)_{lr}\left(YQ^{\perp}\right)_{sn} \times\langle\psi_m\otimes\psi_n, \left(\Gamma + \mathrm{Ex}\left(\gamma\otimes\mathbb{1}_{\mathfrak{h}}\right)\right)(\psi_k\otimes\psi_l)\rangle_{\mathfrak{h}\otimes\mathfrak{h}}.$$

Performing the summation over r and s, leads to

$$\begin{aligned}K &= \sum_{k,l,m,n=1}^{\infty} (QYQ)_{lm} \left(Q^{\perp}YQ^{\perp}\right)_{kn} \\ &\qquad \times \langle \psi_m \otimes \psi_n, (\Gamma + \mathrm{Ex}\,(\gamma \otimes \mathbb{1}_{\mathfrak{h}}))\,(\psi_k \otimes \psi_l)\rangle_{\mathfrak{h}\otimes\mathfrak{h}} \\ &= \sum_{k,l,m,n=1}^{\infty} \left\langle \psi_l \otimes \psi_k, \left(QYQ \otimes Q^{\perp}YQ^{\perp}\right)(\psi_m \otimes \psi_n)\right\rangle_{\mathfrak{h}\otimes\mathfrak{h}} \\ &\qquad \times \langle \psi_m \otimes \psi_n, (\Gamma + \mathrm{Ex}\,(\gamma \otimes \mathbb{1}_{\mathfrak{h}}))\,(\psi_k \otimes \psi_l)\rangle_{\mathfrak{h}\otimes\mathfrak{h}} .\end{aligned}$$

The summations over m and n and finally over k and l yield

$$\begin{aligned}K &= \sum_{k,l=1}^{\infty} \Big\langle \psi_k \otimes \psi_l, \\ &\qquad \left(\mathrm{Ex}\left(QYQ \otimes Q^{\perp}YQ^{\perp}\right)(\Gamma + \mathrm{Ex}\,(\gamma \otimes \mathbb{1}_{\mathfrak{h}}))\right)(\psi_k \otimes \psi_l)\Big\rangle_{\mathfrak{h}\otimes\mathfrak{h}} \\ &= \mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(QYQ \otimes Q^{\perp}YQ^{\perp}\right)(-\Gamma + \mathbb{1}_{\mathfrak{h}} \otimes \gamma)\right),\end{aligned}$$

using the cyclicity of the trace, $\Gamma\,\mathrm{Ex} = -\Gamma$, and $\mathrm{Ex}\,(1_{\mathfrak{h}} \otimes \gamma)\,\mathrm{Ex} = \gamma \otimes \mathbb{1}_{\mathfrak{h}}$.□

Remark 4.16. By changing the definition of $B(r,s)$, it is also possible to treat, for example, $QYQ \otimes QYQ$ similarly. It is, however, important to notice that $\sum_{r,s} B^*(r,s) \otimes B(r,s)$ is in general indefinite. In fact the trace of $B(r,s)$ is vanishing in the considered case and so is the trace of $B^*(r,s) \otimes B(r,s)$. Hence $B^*(r,s) \otimes B(r,s)$ is either indefinite or zero. Furthermore, since $P^{\perp}$ and P commute with γ, we also have $\mathrm{tr}_{\mathfrak{h}}\,(B(r,s)\gamma) = 0$.

A consequence of Lemma 4.15 is a key inequality for proving the estimate on the Remainder and the Main Error Term. This inequality is given in the following lemma.

Lemma 4.17. *Let $X \in \mathcal{B}(\mathfrak{h})$ be an orthogonal projection, and P and $P^{\perp}$ be as defined in (4.36), respectively. Assume that (γ, Γ) is admissible and fulfills the G-condition. Then*

$$\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(PXP \otimes P^{\perp}XP^{\perp}\right)\Gamma\right) \le 4\,\mathrm{tr}_{\mathfrak{h}}\,(X\gamma)\,\mathrm{tr}_{\mathfrak{h}}\left(X\left(\gamma - \gamma^2\right)\right). \tag{4.40}$$

Proof. First we observe that Equation (4.39) with $Y = X$ and $Q = P$ and the G-condition immediately lead to

$$\begin{aligned}0 &\le \sum_{r,s=1}^{\infty} \mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\,((B^*(r,s) \otimes B(r,s))\,(\Gamma + \mathrm{Ex}\,(\gamma \otimes \mathbb{1}_{\mathfrak{h}}))) \\ &= \mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(PXP \otimes P^{\perp}XP^{\perp}\right)(-\Gamma + (\mathbb{1}_{\mathfrak{h}} \otimes \gamma))\right).\end{aligned}$$

Consequently

$$\begin{aligned}\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(PXP \otimes P^{\perp}XP^{\perp}\right)\Gamma\right) &\le \mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(PXP \otimes P^{\perp}XP^{\perp}\right)(\mathbb{1}_{\mathfrak{h}} \otimes \gamma)\right) \\ &= \mathrm{tr}_{\mathfrak{h}}\,(PX)\,\mathrm{tr}_{\mathfrak{h}}\left(P^{\perp}X\gamma\right).\end{aligned}$$

Secondly we permute the arguments in the trace cyclically and use that γ is trace class and PX and $P^\perp X$ are bounded. Then we apply (4.37) to estimate the projections:

$$\begin{aligned}\operatorname{tr}_{\mathfrak{h}}(PX)\operatorname{tr}_{\mathfrak{h}}\left(P^\perp X\gamma\right) &= \operatorname{tr}_{\mathfrak{h}}(XPX)\operatorname{tr}_{\mathfrak{h}}\left(X\sqrt{\gamma}P^\perp\sqrt{\gamma}X\right)\\ &\leq 4\operatorname{tr}_{\mathfrak{h}}(X\gamma)\operatorname{tr}_{\mathfrak{h}}\left(X\left(\gamma-\gamma^2\right)\right)\end{aligned}$$

since $\gamma P^\perp = \sqrt{\gamma}P^\perp\sqrt{\gamma}$. □

Remark 4.18. Since $\operatorname{tr}_{\mathfrak{h}\otimes\mathfrak{h}}((A\otimes B)\Gamma) = \operatorname{tr}_{\mathfrak{h}\otimes\mathfrak{h}}((B\otimes A)\Gamma)$ for any $A, B \in \mathcal{B}(\mathfrak{h})$, we also have

$$\operatorname{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(P^\perp XP^\perp\otimes PXP\right)\Gamma\right) \leq 4\operatorname{tr}_{\mathfrak{h}}(X\gamma)\operatorname{tr}_{\mathfrak{h}}\left(X\left(\gamma-\gamma^2\right)\right).$$

4.2 Estimation of the Remainder

Now we consider the Remainder of Equation (4.38):

$$\begin{aligned}T_{\mathrm{R}} :=& \operatorname{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(P^\perp XP^\perp\otimes P^\perp XP^\perp\right)\Gamma\right)\\ &+4\operatorname{Re}\left\{\operatorname{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(P^\perp XP\otimes P^\perp XP^\perp\right)\Gamma\right)\right\}\\ &+2\operatorname{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(P^\perp XP^\perp\otimes PXP\right)\Gamma\right)+2\operatorname{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(PXP^\perp\otimes P^\perp XP\right)\Gamma\right)\end{aligned}$$

The first three terms, summed up in T_{R_1}, and the last term, denoted by T_{R_2}, are treated separately to derive a lower bound.

Lemma 4.19. *Let $X \in \mathcal{B}(\mathfrak{h})$ be an orthogonal projection, and P and $P^\perp$ as in Definition 4.11. Assume that (γ, Γ) is admissible and fulfills the G- and P-conditions. Then*

$$\begin{aligned}T_{\mathrm{R}_1} :=& \operatorname{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(P^\perp XP^\perp\otimes P^\perp XP^\perp\right)\Gamma\right)+2\operatorname{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(P^\perp XP^\perp\otimes PXP\right)\Gamma\right)\\ &+4\operatorname{Re}\left\{\operatorname{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(P^\perp XP^\perp\otimes PXP^\perp\right)\Gamma\right)\right\}\\ \geq& -8\operatorname{tr}_{\mathfrak{h}}(X\gamma)\operatorname{tr}_{\mathfrak{h}}\left(X\left(\gamma-\gamma^2\right)\right).\end{aligned}$$

Proof. We use $\operatorname{Re}(\zeta) \geq -|\zeta|$ for any complex number ζ and

$$P^\perp XP\otimes P^\perp XP^\perp = \left(P^\perp X\otimes P^\perp X\right)\left(XP\otimes XP^\perp\right)$$

to infer

$$\begin{aligned}T_{\mathrm{R}_1} =& \operatorname{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(P^\perp XP^\perp\otimes P^\perp XP^\perp\right)\Gamma\right)+2\operatorname{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(PXP\otimes P^\perp XP^\perp\right)\Gamma\right)\\ &+4\operatorname{Re}\left\{\operatorname{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(P^\perp XP\otimes P^\perp XP^\perp\right)\Gamma\right)\right\}\\ \geq& \operatorname{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(P^\perp XP^\perp\otimes P^\perp XP^\perp\right)\Gamma\right)+2\operatorname{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(PXP\otimes P^\perp XP^\perp\right)\Gamma\right)\\ &-4\left|\operatorname{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(P^\perp X\otimes P^\perp X\right)\left(XP\otimes XP^\perp\right)\Gamma\right)\right|.\end{aligned}$$

Because $(A, B) := \mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\,(A^* B\,\Gamma)$ defines a positive semi-definite Hermitian form on $\mathcal{B}(\mathfrak{h}\otimes\mathfrak{h})$ due to $\Gamma \geq 0$, which is the P-condition, the Cauchy–Schwarz inequality,

$$|(A, B)| \leq (A, A)^{\frac{1}{2}}\,(B, B)^{\frac{1}{2}}\,, \tag{4.41}$$

holds, and we obtain

$$\begin{aligned} T_{\mathrm{R}_1} \geq\, & \mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(P^\perp X P^\perp \otimes P^\perp X P^\perp\right)\Gamma\right) + 2\,\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(PXP \otimes P^\perp X P^\perp\right)\Gamma\right) \\ & - 4\Big[\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(P^\perp X P^\perp \otimes P^\perp X P^\perp\right)\Gamma\right)\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(PXP \otimes P^\perp X P^\perp\right)\Gamma\right)\Big]^{\frac{1}{2}}. \end{aligned}$$

As $x^2 - 4bx \geq -4b^2$ for $x := \left(\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(P^\perp X P^\perp \otimes P^\perp X P^\perp\right)\Gamma\right)\right)^{\frac{1}{2}}$ and $b := \left(\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(PXP \otimes P^\perp X P^\perp\right)\Gamma\right)\right)^{\frac{1}{2}}$, we then easily conclude

$$\begin{aligned} T_{\mathrm{R}_1} &\geq -4\,\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(PXP \otimes P^\perp X P^\perp\right)\Gamma\right) + 2\,\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(PXP \otimes P^\perp X P^\perp\right)\Gamma\right) \\ &= -2\,\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(PXP \otimes P^\perp X P^\perp\right)\Gamma\right). \end{aligned}$$

The proof is completed by using Inequality (4.40):

$$\begin{aligned} T_{\mathrm{R}_1} &\geq -2\,\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(PXP \otimes P^\perp X P^\perp\right)\Gamma\right) \\ &\geq -8\,\mathrm{tr}_{\mathfrak{h}}\,(X\gamma)\,\mathrm{tr}_{\mathfrak{h}}\left(X\left(\gamma - \gamma^2\right)\right). \end{aligned}$$

□

The estimate of $T_{\mathrm{R}_2} := -2\,\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(P^\perp X P \otimes PXP^\perp\right)\Gamma\right)$ is addressed in the next lemma.

Lemma 4.20. *Let $X = X^* = X^2 \in \mathcal{B}(\mathfrak{h})$, and P and $P^\perp$ as defined in (4.36). Assume that (γ, Γ) is admissible and fulfills the G- and P-conditions. Then*

$$\begin{aligned} T_{\mathrm{R}_2} &= -2\,\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(P^\perp X P \otimes PXP^\perp\right)\Gamma\right) \\ &\geq -8\,\mathrm{tr}_{\mathfrak{h}}\,(X\gamma)\,\mathrm{tr}_{\mathfrak{h}}\left(X\left(\gamma - \gamma^2\right)\right). \end{aligned} \tag{4.42}$$

Proof. Estimating the l.h.s. and afterwards applying the Cauchy–Schwarz inequality (4.41) yields

$$\begin{aligned} & -2\,\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(P^\perp X P \otimes PXP^\perp\right)\Gamma\right) \\ &\quad \geq -2\left|\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(P^\perp X P \otimes PXP^\perp\right)\Gamma\right)\right| \\ &\quad \geq -2\Big[\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(P^\perp X P^\perp \otimes PXP\right)\Gamma\right)\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(PXP \otimes P^\perp X P^\perp\right)\Gamma\right)\Big]^{\frac{1}{2}} \\ &\quad = -2\,\mathrm{tr}_{\mathfrak{h}}\left(\left(PXP \otimes P^\perp X P^\perp\right)\Gamma\right). \end{aligned} \tag{4.43}$$

Again the assertion (4.42) follows from (4.40). □

Summing up the results, we obtain the following estimate of the Remainder directly from Lemmas 4.19 and 4.20.

Theorem 4.21 (Estimation of the Remainder). *Let $X \in \mathcal{B}(\mathfrak{h})$ be an orthogonal projection, and P and $P^\perp$ the orthogonal projections defined in (4.36). Assume that (γ, Γ) is admissible and fulfills the G- and P-conditions. Then*

$$T_R \geq -16 \, \mathrm{tr}_\mathfrak{h} \, (X\gamma) \, \mathrm{tr}_\mathfrak{h} \left(X \left(\gamma - \gamma^2 \right) \right).$$

4.3 Estimation of the Main Error Term

The main error in Theorem 4.7 results from estimating

$$T_{\mathrm{MET}} = 2 \; \mathrm{Re} \left\{ \mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}} \left(\left(P^\perp X P \otimes P^\perp X P \right) \Gamma \right) \right\}. \tag{4.44}$$

A key observation is that any term of the form $A \otimes B \in \mathcal{B}(\mathfrak{h} \otimes \mathfrak{h})$ or $\mathrm{Ex}\,(A \otimes B) \in \mathcal{B}(\mathfrak{h} \otimes \mathfrak{h})$ can be added to Γ in (4.44) without changing the value of T_{MET} provided A and B commute with $P^\perp$ and P. Therefore we can consider

$$T_{\mathrm{MET}} = 2 \; \mathrm{Re} \left\{ \mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}} \left(\left(P^\perp X P \otimes P^\perp X P \right) (\Gamma + \mathrm{Ex}\,(\gamma \otimes \mathbb{1}_\mathfrak{h})) \right) \right\}$$

instead. This expression is estimated using a version of the Cauchy–Schwarz inequality given in the next lemma.

Lemma 4.22. *Let $X = X^* = X^2 \in \mathcal{B}(fh)$, and P and $P^\perp$ be as defined in* (4.36). *Assume that (γ, Γ) is admissible and fulfills the G-condition. Then*

$$\begin{aligned} &\mathrm{Re} \left\{ \mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}} \left(\left(P^\perp X P \otimes P^\perp X P \right) (\Gamma + \mathrm{Ex}\,(\gamma \otimes \mathbb{1}_\mathfrak{h})) \right) \right\} \\ &\qquad \geq - \left(\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}} \left(\left(P X P^\perp \otimes P^\perp X P \right) (\Gamma + \mathrm{Ex}\,(\gamma \otimes \mathbb{1}_\mathfrak{h})) \right) \right)^{\frac{1}{2}} \\ &\qquad\qquad \times \left(\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}} \left(\left(P^\perp X P \otimes P X P^\perp \right) (\Gamma + \mathrm{Ex}\,(\gamma \otimes \mathbb{1}_\mathfrak{h})) \right) \right)^{\frac{1}{2}}. \end{aligned} \tag{4.45}$$

Proof. We define

$$(A, B) := \mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}} \left((A^* \otimes B) \left(\Gamma + \mathrm{Ex}\,(\gamma \otimes \mathbb{1}_\mathfrak{h}) \right) \right)$$

on $\mathcal{B}(\mathfrak{h}) \times \mathcal{B}(\mathfrak{h})$ and observe that $(\cdot\,,\cdot)$ defines a Hermitian form on $\mathcal{B}(\mathfrak{h}) \times \mathcal{B}(\mathfrak{h})$ because

$$\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}} \left((B^* \otimes A) \, \Gamma \right) = \mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}} \left((A \otimes B^*) \, \Gamma \right) = \overline{\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}} \left((A^* \otimes B) \, \Gamma \right)}$$

and

$$\begin{aligned} \mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}} \left((B^* \otimes A) \, \mathrm{Ex}\,(\gamma \otimes \mathbb{1}_\mathfrak{h}) \right) &= \mathrm{tr}_\mathfrak{h} \, (B^* A \, \gamma) = \overline{\mathrm{tr}_\mathfrak{h} \, (A^* B \, \gamma)} \\ &= \overline{\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}} \left((A^* \otimes B) \, \mathrm{Ex}\,(\gamma \otimes \mathbb{1}_\mathfrak{h}) \right)}. \end{aligned}$$

Furthermore $(\cdot\,,\cdot)$ is positive semi-definite since

$$\begin{aligned} (A, A) &= \mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}} \left((A^* \otimes A) \left(\Gamma + \mathrm{Ex}\,(\gamma \otimes \mathbb{1}_\mathfrak{h}) \right) \right) \\ &\geq \left| \mathrm{tr}_\mathfrak{h} \, (A\gamma) \right|^2 \geq 0 \end{aligned}$$

by the G-condition. Hence the Cauchy–Schwarz inequality

$$|(A,B)| \leq (A,A)^{\frac{1}{2}} (B,B)^{\frac{1}{2}}$$

holds true. Applying this with $A^* := B := P^\perp X P$, we obtain the asserted estimate (4.45):

$$\begin{aligned}
\mathrm{Re}&\left\{\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(P^\perp XP \otimes P^\perp XP\right)(\Gamma + \mathrm{Ex}(\gamma \otimes \mathbb{1}_\mathfrak{h}))\right)\right\} \\
&= \mathrm{Re}\left\{(A^*,A)\right\} \geq -\left|(A^*,A)\right| \geq -(A^*,A^*)^{\frac{1}{2}}(A,A)^{\frac{1}{2}} \\
&= -\left(\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(PXP^\perp \otimes P^\perp XP\right)(\Gamma + \mathrm{Ex}(\gamma \otimes \mathbb{1}_\mathfrak{h}))\right)\right)^{\frac{1}{2}} \\
&\qquad \times \left(\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(P^\perp XP \otimes PXP^\perp\right)(\Gamma + \mathrm{Ex}(\gamma \otimes \mathbb{1}_\mathfrak{h}))\right)\right)^{\frac{1}{2}}. \quad \square
\end{aligned}$$

Now the Main Error Term can be estimated.

Theorem 4.23 (Estimation of the Main Error Term). *Let $X \in \mathcal{B}(\mathfrak{h})$ be an orthogonal projection, and P and $P^\perp$ the projections from Definition 4.11. Assume that (γ, Γ) is admissible and fulfills the G- and P-conditions. Then*

$$T_{\mathrm{MET}} \geq -2\,\mathrm{tr}_\mathfrak{h}(X\gamma)\left[8\,\mathrm{tr}_\mathfrak{h}\left(X\left(\gamma-\gamma^2\right)\right)\left(1 + 4\,\mathrm{tr}_\mathfrak{h}\left(X\left(\gamma-\gamma^2\right)\right)\right)\right]^{\frac{1}{2}}.$$

Proof. We rewrite T_{MET} adding the necessary exchange term to allow for an application of Lemma 4.22:

$$\begin{aligned}
T_{\mathrm{MET}} &= 2\,\mathrm{Re}\left\{\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(P^\perp XP \otimes P^\perp XP\right)\Gamma\right)\right\} \\
&= 2\,\mathrm{Re}\left\{\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(P^\perp XP \otimes P^\perp XP\right)(\Gamma + \mathrm{Ex}(\gamma \otimes \mathbb{1}_\mathfrak{h}))\right)\right\} \\
&\geq -2\left(\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(PXP^\perp \otimes P^\perp XP\right)(\Gamma + \mathrm{Ex}(\gamma \otimes \mathbb{1}_\mathfrak{h}))\right)\right)^{\frac{1}{2}} \\
&\qquad \times \left(\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(P^\perp XP \otimes PXP^\perp\right)(\Gamma + \mathrm{Ex}(\gamma \otimes \mathbb{1}_\mathfrak{h}))\right)\right)^{\frac{1}{2}}.
\end{aligned}$$

Note that $\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(PXP^\perp \otimes P^\perp XP\right)\Gamma\right) = \mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(P^\perp XP \otimes PXP^\perp\right)\Gamma\right)$ is already estimated in (4.43). Together with (4.40) we obtain

$$\begin{aligned}
\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(PXP^\perp \otimes P^\perp XP\right)\Gamma\right) &\leq \mathrm{tr}_\mathfrak{h}\left(\left(PXP \otimes P^\perp XP^\perp\right)\Gamma\right) \\
&\leq 4\mathrm{tr}_\mathfrak{h}(X\gamma)\,\mathrm{tr}_\mathfrak{h}\left(X\left(\gamma-\gamma^2\right)\right).
\end{aligned}$$

The two exchange terms are treated separately. Using $P^\perp, P \leq \mathbb{1}_\mathfrak{h}$, we find

$$\begin{aligned}
\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(PXP^\perp \otimes P^\perp XP\right)\mathrm{Ex}(\gamma \otimes \mathbb{1}_\mathfrak{h})\right) &= \mathrm{tr}_\mathfrak{h}\left(P^\perp XP\gamma PXP^\perp\right) \\
&= \mathrm{tr}_\mathfrak{h}\left(P^\perp X\sqrt{\gamma}P\sqrt{\gamma}XP^\perp\right) \\
&\leq \mathrm{tr}_\mathfrak{h}(X\gamma),
\end{aligned}$$

and

$$\begin{aligned}\operatorname{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(P^{\perp}XP\otimes PXP^{\perp}\right)\operatorname{Ex}\left(\gamma\otimes\mathbb{1}_{\mathfrak{h}}\right)\right) &= \operatorname{tr}_{\mathfrak{h}}\left(PXP^{\perp}\gamma P^{\perp}XP\right)\\ &= \operatorname{tr}_{\mathfrak{h}}\left(XPXXP^{\perp}\gamma P^{\perp}X\right)\\ &\leq \operatorname{tr}_{\mathfrak{h}}\left(XPX\right)\operatorname{tr}_{\mathfrak{h}}\left(XP^{\perp}\gamma P^{\perp}X\right)\\ &\leq 4\operatorname{tr}_{\mathfrak{h}}\left(X\gamma\right)\operatorname{tr}_{\mathfrak{h}}\left(X\left(\gamma-\gamma^{2}\right)\right)\end{aligned}$$

where cyclic permutation in the argument of the trace is used together with $X = X^2$, $\left(P^{\perp}\right)^2 = P^{\perp}$, and $P^2 = P$ to expand the argument of the trace. Then $XPX \geq 0$ and $XP^{\perp}\gamma P^{\perp}X \geq 0$ yield the estimate $XPX \leq \mathbb{1}_{\mathfrak{h}}\operatorname{tr}_{\mathfrak{h}}(XPX)$. Afterwards Inequalities (4.37) can be applied. Merging the results, we arrive at the assertion. □

4.4 Estimation of the Main Part

In this subsection it is shown that the remaining terms of (4.38),

$$\begin{aligned}T_{\mathrm{MP}} = &\operatorname{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(PXP\otimes PXP\right)\Gamma\right) + 4\operatorname{Re}\left\{\operatorname{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(PXP^{\perp}\otimes PXP\right)\Gamma\right)\right\}\\ &+ 4\operatorname{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(PXP^{\perp}\otimes P^{\perp}XP\right)\Gamma\right),\end{aligned}$$

are large enough to cover the Hartree–Fock part

$$\operatorname{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(X\otimes X\right)\left(\mathbb{1}_{\mathfrak{h}\otimes\mathfrak{h}} - \operatorname{Ex}\right)\left(\gamma\otimes\gamma\right)\right)$$

in (4.34). Due to this we call this terms the Main Part. As mentioned, the Main Part was extended by an additional term. This extension allows for the following observation.

Lemma 4.24. *Let $X \in \mathcal{B}(\mathfrak{h})$ be an orthogonal projection, and P and $P^{\perp}$ the orthogonal projection defined in (4.36). Then*

$$T_{\mathrm{MP}} = \operatorname{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(PX\left(P+2P^{\perp}\right)\otimes\left(P+2P^{\perp}\right)XP\right)\Gamma\right). \tag{4.46}$$

Proof. Expanding the parentheses on the right side leads to the assertion by using $\operatorname{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(A\otimes B\right)\Gamma\right) = \operatorname{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(B\otimes A\right)\Gamma\right)$. □

For $A := \left(P+2P^{\perp}\right)XP$ we have $T_{\mathrm{MP}} = \operatorname{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(A^{*}\otimes A\right)\Gamma\right)$. This provides the use of the G-condition.

Theorem 4.25 (Main Part versus Hartree–Fock). *Let X, P, and $P^{\perp} \in \mathcal{B}(\mathfrak{h})$ be three orthogonal projection where the later two are defined as in (4.11). Assume that (γ, Γ) is admissible and fulfills the G-condition. Then*

$$\begin{aligned}T_{\mathrm{MP}} - &\operatorname{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left(\left(X\otimes X\right)\left(\mathbb{1}_{\mathfrak{h}} - \operatorname{Ex}\right)\left(\gamma\otimes\gamma\right)\right)\\ &\geq -22\operatorname{tr}_{\mathfrak{h}}\left(X\gamma\right)\operatorname{tr}_{\mathfrak{h}}\left(X\left(\gamma-\gamma^{2}\right)\right).\end{aligned} \tag{4.47}$$

Proof. The proof is split into two parts. In the first part the trace of the Hartree–Fock part is calculated. In the second part the Main Part is estimated by applying the G-condition with $A := \left(P + 2P^{\perp}\right) XP$.

a) As in (4.35) the trace of the Hartree–Fock part can be written as

$$\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}} \left((X \otimes X) \left(\mathbb{1}_{\mathfrak{h}\otimes\mathfrak{h}} - \mathrm{Ex}\right) (\gamma \otimes \gamma) \right) = \left(\mathrm{tr}_{\mathfrak{h}} (X\gamma)\right)^2 - \mathrm{tr}_{\mathfrak{h}} (X\gamma X\gamma) .$$

b) Owing to Lemma 4.24, the G-condition can be applied directly on the Main Part:

$$\begin{aligned} T_{\mathrm{MP}} &= \mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}} \left(\left(PX \left(P + 2P^{\perp}\right) \otimes \left(P + 2P^{\perp}\right) XP \right) \Gamma \right) \\ &\geq \left| \mathrm{tr}_{\mathfrak{h}} \left(PX \left(P + 2P^{\perp}\right) \gamma \right) \right|^2 \\ &\quad - \mathrm{tr}_{\mathfrak{h}} \left(PX \left(P + 2P^{\perp}\right) \gamma \left(P + 2P^{\perp}\right) XP \right) . \end{aligned}$$

Due to cyclic permutation $[\gamma, P] = \left[\gamma, P^{\perp}\right] = 0$ and $P^{\perp}P = PP^{\perp} = 0$ some traces vanish. The result is

$$\begin{aligned} T_{\mathrm{MP}} &\geq \left|\mathrm{tr}_{\mathfrak{h}} (PX\gamma)\right|^2 - \mathrm{tr}_{\mathfrak{h}} (XPXP\gamma) - 4\,\mathrm{tr}_{\mathfrak{h}} \left(XPXP^{\perp}\gamma\right) \\ &\geq \left(\mathrm{tr}_{\mathfrak{h}} (PX\gamma)\right)^2 - \mathrm{tr}_{\mathfrak{h}} (PX\gamma X) - 4\,\mathrm{tr}_{\mathfrak{h}} (XP)\,\mathrm{tr}_{\mathfrak{h}} \left(XP^{\perp}\gamma\right) . \end{aligned}$$

$\mathrm{tr}_{\mathfrak{h}} (XPXP\gamma) = \mathrm{tr}_{\mathfrak{h}} \left(PX\sqrt{\gamma}P\sqrt{\gamma}XP\right) \leq \mathrm{tr}_{\mathfrak{h}} (PX\gamma X)$ is implied by $[P, \gamma] = 0$ together with $P \leq \mathbb{1}_{\mathfrak{h}}$. The application of $XP \leq \mathbb{1}_{\mathfrak{h}}\mathrm{tr}_{\mathfrak{h}} (XP)$ is possible in the last trace since, on the one hand, $\mathrm{tr}_{\mathfrak{h}} \left(XPXP^{\perp}\gamma\right) = \mathrm{tr}_{\mathfrak{h}} \left(XPXXP^{\perp}\gamma X\right)$ and, on the other hand, $XP^{\perp}\gamma X = \left|XP^{\perp}\sqrt{\gamma}\right|^2 \geq 0$ together with $XPX \geq 0$.

Before adding up the estimates, we note that

$$\mathrm{tr}_{\mathfrak{h}} \left(P^{\perp}X\gamma X\gamma\right) = \mathrm{tr}_{\mathfrak{h}} \left(\sqrt{\gamma}X\sqrt{\gamma}P^{\perp}\sqrt{\gamma}X\sqrt{\gamma}\right) \geq 0$$

and

$$\begin{aligned} &\left(\mathrm{tr}_{\mathfrak{h}} (X\gamma)\right)^2 - \left(\mathrm{tr}_{\mathfrak{h}} (PX\gamma)\right)^2 \\ &\qquad = \left(\mathrm{tr}_{\mathfrak{h}} (X\gamma) + \mathrm{tr}_{\mathfrak{h}} (PX\gamma)\right)\left(\mathrm{tr}_{\mathfrak{h}} (X\gamma) - \mathrm{tr}_{\mathfrak{h}} (PX\gamma)\right) \\ &\qquad = \left(\mathrm{tr}_{\mathfrak{h}} (X\gamma) + \mathrm{tr}_{\mathfrak{h}} (PX\gamma)\right)\mathrm{tr}_{\mathfrak{h}} \left(P^{\perp}X\gamma\right) . \end{aligned} \tag{4.48}$$

Furthermore $\mathrm{tr}_{\mathfrak{h}} (XP)\,\mathrm{tr}_{\mathfrak{h}} \left(XP^{\perp}\gamma\right) \leq 4\,\mathrm{tr}_{\mathfrak{h}} (X\gamma)\,\mathrm{tr}_{\mathfrak{h}} \left(X\left(\gamma - \gamma^2\right)\right)$. These results can now be applied together with a) and b) to the l.h.s. of (4.47):

$$\begin{aligned} &T_{\mathrm{MP}} - \mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}} \left((X \otimes X) \left(\mathbb{1}_{\mathfrak{h}\otimes\mathfrak{h}} - \mathrm{Ex}\right) (\gamma \otimes \gamma) \right) \\ &\quad \geq - \left(\left(\mathrm{tr}_{\mathfrak{h}} (X\gamma)\right)^2 - \left(\mathrm{tr}_{\mathfrak{h}} (PX\gamma)\right)^2 \right) + \mathrm{tr}_{\mathfrak{h}} (X\gamma X\gamma) - \mathrm{tr}_{\mathfrak{h}} (PX\gamma X) \\ &\qquad - 16\,\mathrm{tr}_{\mathfrak{h}} (X\gamma)\,\mathrm{tr}_{\mathfrak{h}} \left(X\left(\gamma - \gamma^2\right)\right) . \end{aligned}$$

At this point we use (4.48), $\mathrm{tr}_{\mathfrak{h}}(X\gamma X\gamma) = \mathrm{tr}_{\mathfrak{h}}\left(PX\gamma X\gamma + P^{\perp}X\gamma X\gamma\right)$, and rearrange:

$$\begin{aligned} T_{\mathrm{MP}} &- \mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left((X\otimes X)\left(\mathbb{1}_{\mathfrak{h}\otimes\mathfrak{h}} - \mathrm{Ex}\right)(\gamma\otimes\gamma)\right) \\ &\geq -\left(\mathrm{tr}_{\mathfrak{h}}(X\gamma) + \mathrm{tr}_{\mathfrak{h}}(PX\gamma)\right)\mathrm{tr}_{\mathfrak{h}}\left(P^{\perp}X\gamma\right) \\ &\quad - \mathrm{tr}_{\mathfrak{h}}\left(PX\gamma X\left(\mathbb{1}_{\mathfrak{h}} - \gamma\right)\right) + \mathrm{tr}_{\mathfrak{h}}\left(P^{\perp}X\gamma X\gamma\right) \\ &\quad - 16\,\mathrm{tr}_{\mathfrak{h}}(X\gamma)\,\mathrm{tr}_{\mathfrak{h}}\left(X\left(\gamma-\gamma^2\right)\right). \end{aligned}$$

With $P \leq \mathbb{1}_{\mathfrak{h}}$, $P^{\perp} \leq 2\left(\mathbb{1}_{\mathfrak{h}} - \gamma\right)$, and $\mathrm{tr}_{\mathfrak{h}}\left(P^{\perp}X\gamma X\gamma\right) \geq 0$ we then obtain

$$\begin{aligned} T_{\mathrm{MP}} &- \mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left((X\otimes X)\left(\mathbb{1}_{\mathfrak{h}} - \mathrm{Ex}\right)(\gamma\otimes\gamma)\right) \\ &\geq -4\,\mathrm{tr}_{\mathfrak{h}}(X\gamma)\,\mathrm{tr}_{\mathfrak{h}}\left(X\left(\gamma-\gamma^2\right)\right) - \mathrm{tr}_{\mathfrak{h}}\left(PX\gamma X\left(\mathbb{1}_{\mathfrak{h}} - \gamma\right)\right) \\ &\quad - 16\,\mathrm{tr}_{\mathfrak{h}}(X\gamma)\,\mathrm{tr}_{\mathfrak{h}}\left(X\left(\gamma-\gamma^2\right)\right). \end{aligned}$$

We can apply the inequality $X\gamma X \leq \mathbb{1}_{\mathfrak{h}\otimes\mathfrak{h}}\mathrm{tr}_{\mathfrak{h}}(X\gamma X)$ since $X\gamma X \geq 0$, $\mathrm{tr}_{\mathfrak{h}}\left(PX\gamma X\left(\mathbb{1}_{\mathfrak{h}} - \gamma\right)\right) = \mathrm{tr}_{\mathfrak{h}}\left(X\gamma XX\left(\mathbb{1}_{\mathfrak{h}} - \gamma\right)PX\right)$, and $X\left(\mathbb{1}_{\mathfrak{h}} - \gamma\right)PX = \left|X\sqrt{\mathbb{1}_{\mathfrak{h}} - \gamma}P\right|^2 \geq 0$, and obtain

$$\begin{aligned} T_{\mathrm{MP}} &- \mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left((X\otimes X)\left(\mathbb{1}_{\mathfrak{h}\otimes\mathfrak{h}} - \mathrm{Ex}\right)(\gamma\otimes\gamma)\right) \\ &\geq -20\,\mathrm{tr}_{\mathfrak{h}}(X\gamma)\,\mathrm{tr}_{\mathfrak{h}}\left(X\left(\gamma-\gamma^2\right)\right) - \mathrm{tr}_{\mathfrak{h}}(X\gamma X)\,\mathrm{tr}_{\mathfrak{h}}\left(X\left(\mathbb{1}_{\mathfrak{h}} - \gamma\right)PX\right) \\ &\geq -20\,\mathrm{tr}_{\mathfrak{h}}(X\gamma)\,\mathrm{tr}_{\mathfrak{h}}\left(X\left(\gamma-\gamma^2\right)\right) - 2\,\mathrm{tr}_{\mathfrak{h}}(X\gamma)\,\mathrm{tr}_{\mathfrak{h}}\left(X\left(\gamma-\gamma^2\right)\right) \\ &= -22\,\mathrm{tr}_{\mathfrak{h}}(X\gamma)\,\mathrm{tr}_{\mathfrak{h}}\left(X\left(\gamma-\gamma^2\right)\right). \end{aligned}$$

The last inequality follows from $P \leq 2\gamma$. □

Finally the proof of Theorem 4.7 is completed by the estimations of the Remainder in Theorem 4.21, of the Main Error Term in Theorem 4.23, and of $T_{\mathrm{MP}} - \mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left((X\otimes X)\left(\mathbb{1}_{\mathfrak{h}\otimes\mathfrak{h}} - \mathrm{Ex}\right)(\gamma\otimes\gamma)\right)$ in Theorem 4.25. In each of these theorems the G-condition is used to generate bounds. The P-condition is only applied to provide the use of the Cauchy–Schwarz inequality. In the end it is remarkable that the Q-condition is not needed for the proof of the correlation estimate.

5 Summary

We obtained several results in the last section which are merged in the main theorem, Theorem 4.7:

$$\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left((X\otimes X)\left(\Gamma - \left(\mathbb{1}_{\mathfrak{h}\otimes\mathfrak{h}} - \mathrm{Ex}\right)(\gamma\otimes\gamma)\right)\right) \geq -\mathrm{tr}_{\mathfrak{h}}(X\gamma),$$

$$T_{\mathrm{R}} \geq -16\,\mathrm{tr}_{\mathfrak{h}}(X\gamma)\,\mathrm{tr}_{\mathfrak{h}}\left(X\left(\gamma-\gamma^2\right)\right),$$

$$T_{\mathrm{MET}} \geq -2\,\mathrm{tr}_{\mathfrak{h}}(X\gamma)\left[8\,\mathrm{tr}_{\mathfrak{h}}\left(X\left(\gamma-\gamma^2\right)\right)\left(1 + 4\,\mathrm{tr}_{\mathfrak{h}}\left(X\left(\gamma-\gamma^2\right)\right)\right)\right]^{\frac{1}{2}},$$

$$
\begin{aligned}
T_{\mathrm{MP}} - \mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}} \left((X \otimes X) \left(\mathbb{1}_{\mathfrak{h}\otimes\mathfrak{h}} - \mathrm{Ex} \right) (\gamma \otimes \gamma) \right) \\
\geq -22\, \mathrm{tr}_{\mathfrak{h}} (X\gamma)\, \mathrm{tr}_{\mathfrak{h}} \left(X \left(\gamma - \gamma^2 \right) \right).
\end{aligned}
$$

Denoting $b := \mathrm{tr}_{\mathfrak{h}} (X\gamma)$ and $a := \sqrt{\mathrm{tr}_{\mathfrak{h}} (X (\gamma - \gamma^2))}$ we can rewrite the estimates for $\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}} \left((X \otimes X) \Gamma^{(\mathrm{T})} \right)$ with $\Gamma^{(\mathrm{T})} := \Gamma - (\mathbb{1}_{\mathfrak{h}\otimes\mathfrak{h}} - \mathrm{Ex}) (\gamma \otimes \gamma)$ as

$$
\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}} \left((X \otimes X) \Gamma^{(\mathrm{T})} \right) \geq -b \min \left\{ 1;\ a \left(38a + 2\sqrt{8 + 32a^2} \right) \right\}. \tag{4.49}
$$

A suitable choice of $a \leq b$ in Inequality (4.49) leads to the following correlation estimation.

Theorem 4.26 (Optimization of Correlation Inequality). *Let $X \in \mathcal{B}(\mathfrak{h})$ be an orthogonal projection, and P and $P^{\perp}$ the orthogonal projections given in (4.36). Assume that (γ, Γ) is admissible and fulfills the G- and P-conditions. Then*

$$
\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}} \left((X \otimes X) \Gamma^{(\mathrm{T})} \right) \geq -\mathrm{tr}_{\mathfrak{h}} (X\gamma) \min \left\{ 1;\ 10 \sqrt{\mathrm{tr}_{\mathfrak{h}} (X (\gamma - \gamma^2))} \right\}.
$$

Proof. The minimum of the r.h.s. of (4.49) is $a \left(38a + 2\sqrt{8 + 32a^2} \right)$ for $0 < a \leq 1/\sqrt{94}$ and thus $1/a \geq \left(38a + 2\sqrt{8 + 32a^2} \right)$. Since the term $\left(38a + 2\sqrt{8 + 32a^2} \right)$ is monotonously increasing in a, we find

$$
\left(38a + 2\sqrt{8 + 32a^2} \right) \leq \sqrt{94} < 10 \tag{4.50}
$$

which implies the assertion. □

Remark 4.27. In Section 4.1 we have split the eigenvalues of γ in eigenvalues which are greater than $1/2$ and lower than or equal to $1/2$. In fact this split turns out to be almost optimal and (4.50) cannot be sharpened by another choice of P and $P^{\perp}$.

Up to the constant (4.50) Theorem 4.26 is exactly the result which was already obtained in [Bac92]. The difference of the constants arises, on the one hand, since the terms of $\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}} \left((X \otimes X) \Gamma^{(\mathrm{T})} \right)$ are differently arranged and, on the other hand, from the fact that in [Bac92] also the Q-condition was used which can be seen implicitly in estimate (68) in [Bac92]. With the result of Theorem 4.26 we can immediately perform the integration in the Fefferman–de la Llave identity according to [Bac92] which leads to an estimate of $\mathrm{tr}_{\mathfrak{h}\otimes\mathfrak{h}} (V (\Gamma - (\mathbb{1}_{\mathfrak{h}\otimes\mathfrak{h}} - \mathrm{Ex})(\gamma \otimes \gamma)))$.

Chapter 5

Representability Conditions by Grassmann Integration

This chapter is the result of a joint work with V. Bach and E. Menge and a version of it will be published separately [BKM13].

1 Introduction

The grand canonical energy (minus pressure) $E_0(\mu) := \inf\left\{\sigma\left\{\mathbb{H} - \mu\widehat{\mathbb{N}}\right\}\right\}$ at sufficiently large chemical potential $\mu \geq 0$ of a quantum system with a Hamiltonian $\mathbb{H}$ and particle number operator $\widehat{\mathbb{N}}$ is given by the Rayleigh–Ritz principle as

$$E_0(\mu) = \inf\left\{\mathrm{tr}_{\wedge\mathcal{H}}\left(\rho^{\frac{1}{2}}\left(\mathbb{H} - \mu\widehat{\mathbb{N}}\right)\rho^{\frac{1}{2}}\right) \,\middle|\, \rho \in DM\right\}. \tag{5.1}$$

The Hamiltonian is assumed to be selfadjoint and to obey stability of matter, i.e., it is bounded below by $-c\widehat{\mathbb{N}}$ for some $c < \infty$ and at most quartic in the creation and annihilation operators [LT75, Thi08]. This is typically the case for models of non-relativistic matter in physics and chemistry. The Pauli principle plays a crucial role for stability of matter to hold true and we thus restrict our attention to fermion systems. On the fermion Fock space $\wedge\mathcal{H}$ over a separable Hilbert space $\mathcal{H}$, the variation on the r.h.s. of (5.1) is over the set

$$DM := \left\{\rho \,\middle|\, \rho \in \mathcal{L}^1_+(\wedge\mathcal{H}),\ \mathrm{tr}_{\wedge\mathcal{H}}(\rho) = 1,\ \left\langle\widehat{\mathbb{N}}^2\right\rangle_\rho < \infty\right\},$$

i.e., density matrices with finite particle number variance. Here the expectation value of an observable $\mathbb{A}$ is

$$\langle\mathbb{A}\rangle_\rho := \mathrm{tr}_{\wedge\mathcal{H}}\left(\rho^{\frac{1}{2}}\mathbb{A}\rho^{\frac{1}{2}}\right).$$

More specifically, if

$$\mathbb{H} - \mu\widehat{\mathbb{N}} = \sum_{k,m} h_{km}c^*(f_k)c(f_m) + \sum_{k,l,m,n} V_{klmn}c^*(f_l)c^*(f_k)c(f_m)c(f_n),$$

then

$$E_0(\mu) = \inf\{\mathcal{E}(\gamma_\rho, \Gamma_\rho) \mid \rho \in DM\} \tag{5.2}$$

where

$$\mathcal{E}(\gamma_\rho, \Gamma_\rho) = \sum_{k,m} h_{km} \langle f_m, \gamma_\rho f_k \rangle_{\mathcal{H}} + \sum_{k,l,m,n} V_{klmn} \langle f_m \otimes f_n, \Gamma_\rho (f_k \otimes f_l) \rangle_{\mathcal{H}\otimes\mathcal{H}}$$

and the one- and two-particle density matrices corresponding to ρ are defined by

$$\langle f, \gamma_\rho g \rangle_{\mathcal{H}} := \langle c^*(g) c(f) \rangle_\rho \quad \text{and}$$
$$\langle f \otimes g, \Gamma_\rho (\tilde{f} \otimes \tilde{g}) \rangle_{\mathcal{H}\otimes\mathcal{H}} := \langle c^*(\tilde{g}) c^*(\tilde{f}) c(f) c(g) \rangle_\rho,$$

respectively, for all $f, g, \tilde{f}, \tilde{g} \in \mathcal{H}$. Note that (5.2) can be rewritten as

$$E_0(\mu) = \inf\{\mathcal{E}(\gamma, \Gamma) \mid (\gamma, \Gamma) \in \mathcal{R}\} \tag{5.3}$$

where

$$\mathcal{R} := \left\{ (\gamma, \Gamma) \in \mathcal{L}^1(\mathcal{H}) \times \mathcal{L}^1(\mathcal{H} \otimes \mathcal{H}) \middle| \exists \rho \in DM : (\gamma, \Gamma) = (\gamma_\rho, \Gamma_\rho) \right\}$$

denotes the set of all representable one- and two-particle density matrices. Equation (5.3) suggests that the search for a minimizing ρ could be drastically simplified if one would find a characterization of all representable reduced density matrices (γ, Γ). This was realized almost fifty years ago [Col63, Erd78b, GP64, Löw55], but such a characterization is still unknown.

The characterization of $E_0(\mu)$ by (5.3) immediately yields lower bounds of the form

$$E_0(\mu) =: E_{\mathcal{R}}(\mu) \geq E_{\mathcal{S}}(\mu) \tag{5.4}$$

for any superset $\mathcal{S}$ of $\mathcal{R}$. For example, the positivity $\langle P_2^* P_2 \rangle_\rho \geq 0$ for all polynomials $P_2 \equiv P_2(c^*, c)$ in the creation and annihilation operators of degree two yields the so-called G-, P-, and Q-conditions on $(\gamma_\rho, \Gamma_\rho)$ [BKM12, Col63, Erd78b, GP64]. Similarly the positivity $\langle P_3^* P_3 + P_3 P_3^* \rangle_\rho \geq 0$ yields the T_1- and generalized T_2-Conditions [Erd78b]. Hence all representable reduced density matrices (γ, Γ) necessarily fulfill the G-, P-, Q-, T_1-, and generalized T_2-conditions, and we have

$$E_{\mathcal{R}}(\mu) \geq E_{\mathcal{S}[G,P,Q,T_1,T_2]}(\mu) \geq E_{\mathcal{S}[G,P,Q]}(\mu) \tag{5.5}$$

since $\mathcal{R} \subseteq \mathcal{S}[G,P,Q,T_1,T_2] \subseteq \mathcal{S}[G,P,Q]$ with

$$\mathcal{S}[X] := \left\{ (\gamma, \Gamma) \in \mathcal{L}^1(\mathcal{H}) \times \mathcal{L}^1(\mathcal{H} \otimes \mathcal{H}) \middle| (\gamma, \Gamma) \text{ fulfills Conditions } X \right\}.$$

We have discussed (5.4)-(5.5) for $\mathcal{S} = \mathcal{S}[G,P]$ in some detail in [BKM12] and refer the reader to that paper and references therein. Furthermore for $\mathcal{S} = \mathcal{S}[G,P,Q,T_1,T_2]$ numerical works show agreement with Full CI computations [CLS06, Maz02, Maz12b, ZBF+04] to high accuracy.

The purpose of the present paper is the reformulation of representability conditions in terms of Grassmann integrals. Such a transcription may possibly yield new viewpoints and hopefully new insights into the representability problem. To this end we introduce a Grassmann algebra $\mathcal{G}_M$ as a finite dimensional complex algebra. The object on $\mathcal{G}_M$ corresponding to a given density matrix is an element of the form $\vartheta^* \star \vartheta$ described in the sequel. Grassmann integration is the basic and most commonly used method (see, e.g., [FKT02, Sal98]) in theoretical physics to compute partition functions of the form

$$Z_{\Gamma,\lambda}(J) := \int \mathrm{D}_\Gamma(\phi)\, \mathrm{e}^{-S_\Gamma + (J,\phi)_\Gamma}$$

as a functional integral with $\mathrm{D}_\Gamma(\phi) := \prod_{x\in\Gamma} \mathrm{d}\phi\,(x)$ with sources $J : \Gamma \to \mathbb{R}$ and an action S_Γ (see [Sal98] for further details).

The derivation of the G-, P-, Q-, T_1-, and generalized T_2-conditions is based on the representation of the trace on $\wedge\mathcal{H}$ in terms of Grassmann integrals and a non-negativity condition of a Grassmann integral, namely

$$\int \mathrm{d}(\overline{\Psi},\Psi)\, \mathrm{e}^{2\left(\overline{\Psi},\Psi\right)} \eta^* \star \eta \geq 0, \tag{5.6}$$

for all $\eta \in \mathcal{G}_M$ where $\int \mathrm{d}(\overline{\Psi},\Psi)$ denotes the Grassmann integration. The star product refers to a product on $\mathcal{G}_M$ and is introduced later. Considering appropriate subspaces of $\mathcal{G}_M$ denoted by $\mathcal{G}_M^{(n)}$, the main results of this paper are the bounds for the one-particle density matrix γ_ϑ:

$$\left\{\forall \mu \in \mathcal{G}_M^{(1)} : \int \mathrm{d}(\overline{\Psi},\Psi)\, \mathrm{e}^{2\left(\overline{\Psi},\Psi\right)} \vartheta^* \star \vartheta \star \mu \geq 0\right\} \Leftrightarrow \{0 \leq \gamma_\vartheta \leq \mathbb{1}_\mathcal{H}\}$$

and the G-, P-, and Q-conditions as conditions for the two-particle density matrix Γ_ϑ:

$$\left\{\forall \mu \in \mathcal{G}_M^{(2)} : \int \mathrm{d}(\overline{\Psi},\Psi)\, \mathrm{e}^{2\left(\overline{\Psi},\Psi\right)} \vartheta^* \star \vartheta \star \mu \geq 0\right\}$$
$$\Leftrightarrow \{0 \leq \gamma_\vartheta \leq \mathbb{1}_\mathcal{H},\ \text{G-, P-, and Q-condition}\}$$

Finally we prove the validity of the T_1- and generalized T_2-condition by Inequality (5.6).

2 Reduced Density Matrices and Representability

Before we elucidate how to derive the G-, P-, Q-, T_1-, and generalized T_2-conditions for the one- and two-particle density matrix (1- and 2-pdm) by Grassmann integration, we give a definition of these first two reduced density matrices. For this purpose we consider a finite-dimensional index set M, an $|M|$-dimensional (one-particle) Hilbert space $(\mathcal{H}, \langle\cdot,\cdot\rangle_\mathcal{H})$, and an arbitrary, but fixed orthonormal basis (ONB) $\{\psi_i\}_{i\in M}$ of $\mathcal{H}$ where $\langle\cdot,\cdot\rangle_\mathcal{H}$ is linear in the second and antilinear in the first argument. Furthermore we introduce the usual fermion creation and annihilation operators on the fermion Fock space $\wedge\mathcal{H}$ over $\mathcal{H}$ given by $c^*(\psi_i) \equiv c_i^*$ and $c(\psi_i) \equiv c_i$ with the canonical anticommutation relations (CAR)

$$\{c(f), c(g)\} = \{c^*(f), c^*(g)\} = 0 \text{ and } \{c(f), c^*(g)\} = \langle f, g\rangle_{\mathcal{H}} \mathbb{1}_{\wedge\mathcal{H}}$$

for all $f, g \in \mathcal{H}$ where $\{A, B\} := AB + BA$ denotes the anticommutator.

The 1-pdm $\gamma_\rho \in \mathcal{L}^1_+(\mathcal{H})$ of a density matrix ρ, i.e., a positive trace class operator on $\wedge\mathcal{H}$ of unit trace ($\mathrm{tr}_{\wedge\mathcal{H}}(\rho) = 1$), is defined by its matrix elements as

$$\langle f, \gamma_\rho g\rangle_{\mathcal{H}} := \mathrm{tr}_{\wedge\mathcal{H}}\left(\rho\, c^*(g)c(f)\right)$$

for any $f, g \in \mathcal{H}$. Likewise the 2-pdm $\Gamma_\rho \in \mathcal{L}^1_+(\mathcal{H}\otimes\mathcal{H})$ of ρ is defined for any $f_1, f_2, g_1, g_2 \in \mathcal{H}$ by

$$\langle f_1 \otimes f_2, \Gamma_\rho(g_1 \otimes g_2)\rangle_{\mathcal{H}\otimes\mathcal{H}} := \mathrm{tr}_{\wedge\mathcal{H}}\left(\rho\, c^*(g_2)c^*(g_1)c(f_1)c(f_2)\right).$$

There are several properties which can be derived directly from the definition of γ_ρ and Γ_ρ:

Lemma 5.1. *Let $\rho \in \mathcal{L}^1_+(\wedge\mathcal{H})$ be a density matrix and $\widehat{\mathbb{N}} := \sum_{k\in M} c_k^* c_k$ the particle number operator with $\left\langle \widehat{\mathbb{N}}^2 \right\rangle_\rho < \infty$. Then the following assertions hold true:*

(i) $\gamma_\rho \in \mathcal{L}^1_+(\mathcal{H})$, $0 \le \gamma_\rho \le \mathbb{1}_{\mathcal{H}}$, $\mathrm{tr}_{\mathcal{H}}(\gamma_\rho) = \left\langle \widehat{\mathbb{N}} \right\rangle_\rho$, $\Gamma_\rho \in \mathcal{L}^1_+(\mathcal{H}\otimes\mathcal{H})$, $0 \le \Gamma_\rho \le \left\langle \widehat{\mathbb{N}} \right\rangle_\rho \mathbb{1}_{\mathcal{H}\otimes\mathcal{H}}$, *and* $\mathrm{tr}_{\mathcal{H}\otimes\mathcal{H}}(\Gamma_\rho) = \left\langle \widehat{\mathbb{N}}\left(\widehat{\mathbb{N}} - \mathbb{1}_{\wedge\mathcal{H}}\right)\right\rangle_\rho$.

(ii) If $\mathrm{ran}(\rho) \subseteq \wedge^{(N)}\mathcal{H}$ for some $N \in \mathbb{N}$, then

$$\langle f, \gamma_\rho g\rangle_{\mathcal{H}} = \frac{1}{N-1} \sum_{k\in M} \langle f \otimes \varphi_k, \Gamma_\rho(g \otimes \varphi_k)\rangle_{\mathcal{H}\otimes\mathcal{H}}$$

holds for all $f, g \in \mathcal{H}$ where $\{\varphi_k\}_{k\in M}$ is an ONB of $\mathcal{H}$. Here $\wedge^{(N)}\mathcal{H}$ denotes the fermion N-particle Fock space.

(iii) Furthermore we have

$$\rho = |c^*(\varphi_1)\cdots c^*(\varphi_N)\Omega\rangle \langle c^*(\varphi_1)\cdots c^*(\varphi_N)\Omega| \;\Leftrightarrow\; \gamma_\rho = \sum_{i=1}^{N} |\varphi_i\rangle\langle\varphi_i|$$

and in this case

$$\Gamma_\rho = \left(\mathbb{1}_{\mathcal{H}\otimes\mathcal{H}} - \mathrm{Ex}\right)\left(\gamma_\rho \otimes \gamma_\rho\right)$$

where the exchange operator Ex *is given by* $\mathrm{Ex}(f \otimes g) := g \otimes f$ *for any $f, g \in \mathcal{H}$ and $\Omega \in \wedge\mathcal{H}$ denotes the vacuum vector.*

For further details we recommend [Bac92, BKM12, Col63, GP64]. A proof can be found in [Bac92]. Beside these properties necessary conditions on (γ, Γ) to be representable were derived in [Col63, Erd78b, GP64]. In particular, the P-, G-, and Q-conditions are given as follows:

- (γ, Γ) fulfills the P-condition $:\Leftrightarrow$ $\Gamma \geq 0$,
- (γ, Γ) fulfills the G-condition $:\Leftrightarrow$ For all $A \in \mathcal{B}(\mathcal{H})$ $\mathrm{tr}_{\mathcal{H}\otimes\mathcal{H}}\left((A^* \otimes A)\left(\Gamma + \mathrm{Ex}\left(\gamma \otimes \mathbb{1}_{\mathcal{H}}\right)\right)\right) \geq \left|\mathrm{tr}_{\mathcal{H}}\left(A\gamma\right)\right|^2$,
- (γ, Γ) fulfills the Q-condition $:\Leftrightarrow$ $\Gamma + \left(\mathbb{1}_{\mathcal{H}\otimes\mathcal{H}} - \mathrm{Ex}\right)\left(\mathbb{1}_{\mathcal{H}} \otimes \mathbb{1}_{\mathcal{H}} - \gamma \otimes \mathbb{1}_{\mathcal{H}} - \mathbb{1}_{\mathcal{H}} \otimes \gamma\right) \geq 0$.

The T_1- and the generalized T_2-condition are more complicated and not given here. For this conditions we refer the reader to [Erd78b] or Subsection 5.3 of this work.

3 Grassmann Algebras

We introduce the Grassmann algebra as the complex algebra generated by elements of the set $\{\overline{\psi}_i, \psi_i\}_{i\in M}$ with $|M| < \infty$ modulo the anticommutation relations specified below. A product on this Grassmann algebra is denoted by $\psi_i \cdot \psi_j \equiv \psi_i\psi_j$ for any two generators. The unity is given as $1 \cdot \psi_i = \psi_i \cdot 1 = \psi_i$ (and in the same manner for $\overline{\psi}_j$). The anticommutation relations given below allow us to find a one-to-one representation of the CAR of fermion creation and annihilation operators in terms of the Grassmann variables. For further details on this well-known material we recommend [CR12, dSP05, Sal98, Tak08]. In this work we use the notation of [dSP05].

Definition 5.2. For an ordered set $I := \{i_1, \ldots, i_m\} \subseteq M$ we write

$$\Psi_I := \psi_{i_1} \cdots \psi_{i_m}, \quad \overline{\Psi}_I := \overline{\psi}_{i_1} \cdots \overline{\psi}_{i_m}.$$

For $I = \emptyset$ we set $\Psi_I = \overline{\Psi}_I = 1$. Denoting the reversely ordered set corresponding to I by I', we write

$$\Psi_{I'} := \psi_{i_m} \cdots \psi_{i_1}.$$

Definition 5.3. Given a set of generators $\{\overline{\psi}_i, \psi_i\}_{i\in M}$ obeying the anticommutation relations

$$\overline{\psi}_i\psi_j + \psi_j\overline{\psi}_i = \overline{\psi}_i\overline{\psi}_j + \overline{\psi}_j\overline{\psi}_i = \psi_i\psi_j + \psi_j\psi_i = 0$$

for any $i, j \in M$, the Grassmann algebra $\mathcal{G}_M$ is defined as

$$\mathcal{G}_M := \mathrm{span}\left\{\overline{\Psi}_I\Psi_J \,\middle|\, I, J \subseteq M\right\}.$$

Introducing the ordinary wedge product we can identify $\mathcal{G}_M$ with the Fock space $\wedge\left(\overline{\mathcal{H}} \oplus \mathcal{H}\right)$ of a Hilbert space $(\mathcal{H}, \langle\cdot,\cdot\rangle_{\mathcal{H}})$ with finite dimension $|M|$. Considering $\mathcal{H}$ as a subset of $\mathcal{G}_M$ we can identify $\{\psi_i\}_{i\in M}$ with a fixed ONB of $\mathcal{H}$ and $\{\overline{\psi}_i\}_{i\in M}$ with the corresponding ONB of $\overline{\mathcal{H}}$, i.e., the space of all continuous linear functionals $\mathcal{H} \to \mathbb{C}$ with $\overline{\psi}_i(\psi_j) := \langle\psi_i, \psi_j\rangle_{\mathcal{H}}$.

Remark 5.4. If $\mathcal{G}_M$ is generated by $\{\overline{\phi}_i, \phi_i\}_{i\in M}$, we emphasize this by using $\mu\left(\overline{\phi}, \phi\right) \in \mathcal{G}_M$ instead of $\mu \in \mathcal{G}_M$. We also use "mixed" generators, e.g.,

$$\mu\left(\overline{\psi}, \phi\right) := \sum_{i,j} \alpha_{ij}\, \overline{\Psi}_{I_i} \Phi_{J_j}$$

with $\alpha_{ij} \in \mathbb{C}$ for any i, j.

Later it is necessary to link the CAR algebra of fermion annihilation and creation operators to a Grassmann algebra. For this purpose a map between $\mathcal{B}(\wedge\mathcal{H})$ and $\mathcal{G}_M$ that is an isomorphism between vector spaces is required. This map is provided below.

Definition 5.5. Let $\mathcal{G}_M$ be generated by $\{\overline{\psi}_i, \psi_i\}_{i\in M}$ and associate $\{\psi_i\}_{i\in M}$ with a fixed ONB of $\mathcal{H}$. For all $z \in \mathbb{C}$ and $m, n \leq |M|$ we define the linear map $\Theta : \mathcal{B}(\wedge\mathcal{H}) \to \mathcal{G}_M$ by $\Theta(z) := z$ and

$$\Theta\left(c^*(\psi_{i_1}) \cdots c^*(\psi_{i_m}) c(\psi_{j_1}) \cdots c(\psi_{j_n})\right) := \overline{\psi}_{i_1} \cdots \overline{\psi}_{i_m} \psi_{j_1} \cdots \psi_{j_n} \tag{5.7}$$

and extension to $\mathcal{B}(\wedge\mathcal{H})$ by linearity.

We emphasize that Θ is not multiplicative. E.g., while

$$\Theta\left(c^*(\psi_1)c(\psi_1)\right) = \overline{\psi}_1\psi_1 = \Theta\left(c^*(\psi_1)\right)\Theta\left(c(\psi_1)\right),$$

we have

$$\begin{aligned}\Theta\left(c(\psi_1)c^*(\psi_1)\right) &= \Theta\left(-c^*(\psi_1)c(\psi_1) + \mathbb{1}_{\wedge\mathcal{H}}\right) \\ &= -\overline{\psi}_1\psi_1 + 1 = \psi_1\overline{\psi}_1 + 1 = \Theta\left(c(\psi_1)\right)\Theta\left(c^*(\psi_1)\right) + 1.\end{aligned}$$

Thus, Equation (5.7) only holds for normal-ordered monomials in creation and annihilation operators, i.e., monomials in which all creation operators are to the left of all annihilation operators.

Definition 5.6. For any $A \in \mathcal{B}(\mathcal{H})$ we set

$$\left(\overline{\Psi}, A\Phi\right) := \sum_{i,j\in M} \left[\overline{\psi}_i(A\psi_j)\right] \overline{\psi}_j \phi_i \in \mathcal{G}_M.$$

Note that $\overline{\psi}_i(A\psi_j) = \langle\psi_i, A\psi_j\rangle_{\mathcal{H}} \in \mathbb{C}$. Furthermore $\left(\overline{\Psi}, A\Phi\right)$ does not depend on the choice of generators of $\mathcal{G}_M$ as can be seen by a unitary change of generators, i.e., $\chi_i := \sum_{j\in M} U_{ij}\psi_j$ for a unitary matrix U. An important case is $A = \mathbb{1}_{\mathcal{H}}$ and we then have $\left(\overline{\Psi}, \Phi\right) = \sum_{i\in M} \overline{\psi}_i\phi_i$. One of the last ingredients for the Grassmann integration is the following:

Definition 5.7. The expression $\mathrm{e}^{\pm\left(\overline{\Psi}, A\Phi\right)} \in \mathcal{G}_M$ is given by

$$\mathrm{e}^{\pm\left(\overline{\Psi}, A\Phi\right)} := \sum_{m=0}^{\infty} \frac{1}{m!}\left[\pm\left(\overline{\Psi}, A\Phi\right)\right]^m.$$

As $\dim(\wedge\mathcal{H}) = 2^{\dim(\mathcal{H})}$, the sum runs only over $0 \leq m \leq 2^{\dim(\mathcal{H})}$.

Remark 5.8. Since $\left(\overline{\Psi},\Phi\right) = \sum_{\alpha\in M}\overline{\psi}_\alpha\phi_\alpha$ and $\overline{\psi}_\alpha\phi_\alpha$ commutes with every element of $\mathcal{G}_M$, we have

$$\mathrm{e}^{\pm\left(\overline{\Psi},\Phi\right)} = \prod_{\alpha\in M}\left(1\pm\overline{\psi}_\alpha\phi_\alpha\right). \tag{5.8}$$

Definition 5.9. For all $i,j\in M$ we define the vector space homomorphisms $\frac{\delta}{\delta\psi_i}, \frac{\delta}{\delta\overline{\psi}_i} : \mathcal{G}_M \to \mathcal{G}_M$ by

$$\frac{\delta}{\delta\psi_i}\psi_j = \frac{\delta}{\delta\overline{\psi}_i}\overline{\psi}_j = \delta_{ij}, \quad \text{and} \quad \frac{\delta}{\delta\psi_i}\overline{\psi}_j = \frac{\delta}{\delta\overline{\psi}_i}\psi_j = 0.$$

Remark 5.10. The set $\left\{\frac{\delta}{\delta\overline{\psi}_i}, \frac{\delta}{\delta\psi_i}\right\}_{i\in M}$ itself generates a Grassmann algebra.

4 Grassmann Integration

Now we are prepared to define the Grassmann integral, which is a linear operator from the Grassmann algebra $\mathcal{G}_M$ to the complex numbers $\mathbb{C}$.

Definition 5.11. The map $\int \mathrm{d}(\overline{\Psi},\Psi) : \mathcal{G}_M \to \mathbb{C}$ is defined by

$$\int \mathrm{d}(\overline{\Psi},\Psi) := \prod_{\alpha\in M}\left(\frac{\delta}{\delta\overline{\psi}_\alpha}\frac{\delta}{\delta\psi_\alpha}\right)$$

and referred to as the Grassmann integral.

Remark 5.12. If the factor $\mathrm{e}^{2\left(\overline{\Psi},\Psi\right)} = \prod_{\alpha\in M}\left(1+2\overline{\psi}_\alpha\psi_\alpha\right)$ is involved in the integration, we use the abbreviation

$$\mathcal{D}(\overline{\Psi},\Psi) := \mathrm{d}(\overline{\Psi},\Psi)\,\mathrm{e}^{2\left(\overline{\Psi},\Psi\right)}.$$

We can always write this exponential as the first factor of the integrand since $\prod_{\alpha\in M}\left(1+2\overline{\psi}_\alpha\psi_\alpha\right)$ commutes with every element of $\mathcal{G}_M$.

In order to state the invariance of the Grassmann integration with respect to a change of generators, we introduce some notations. We write two sets of generators, $\left\{\overline{\psi}_i,\psi_i\right\}_{i\in M}$ and $\{\overline{\chi}_i,\chi_i\}_{i\in M}$, as $2|M|$-component vectors $\underline{a}$ and $\underline{b}$, respectively, where for all $i\in M$

$$a_i := \overline{\psi}_i \text{ and } a_{|M|+i} := \psi_i, \quad \text{and} \quad b_i := \overline{\chi}_i \text{ and } b_{|M|+i} := \chi_i. \tag{5.9}$$

Furthermore we define the entries of the $2|M|$-component vectors $\frac{\delta}{\delta\underline{a}}$ and $\frac{\delta}{\delta\underline{b}}$ by

$$\frac{\delta}{\delta\underline{a}_i} := \frac{\delta}{\delta\overline{\psi}_i} \text{ and } \frac{\delta}{\delta\underline{a}_{|M|+i}} := \frac{\delta}{\delta\psi_i}, \quad \text{and} \quad \frac{\delta}{\delta\underline{b}_i} := \frac{\delta}{\delta\overline{\chi}_i} \text{ and } \frac{\delta}{\delta\underline{b}_{|M|+i}} := \frac{\delta}{\delta\chi_i}.$$

We denote the index set for the introduced vectors by $\widetilde{M}$ and therefore $|\widetilde{M}| = 2|M|$. In this notation the Grassmann integration with respect to $\left\{\overline{\psi}_i,\psi_i\right\}_{i\in M}$ reads

$$(-1)^{\frac{1}{2}|M|(|M|-1)}\prod_{\alpha\in M}\left(\frac{\delta}{\delta\overline{\psi}_\alpha}\frac{\delta}{\delta\psi_\alpha}\right) = \prod_{\alpha\in M}\frac{\delta}{\delta\overline{\psi}_\alpha}\prod_{\alpha\in M}\frac{\delta}{\delta\psi_\alpha} = \prod_{\beta\in\widetilde{M}}\frac{\delta}{\delta\underline{a}_\beta}.$$

Lemma 5.13. *The Grassmann integral does not depend on the choice of the generators. I.e., for $\underline{a}$ and $\underline{b}$ as defined in (5.9), and a transformation defined by*

$$\underline{b} = U\,\underline{a}$$

where U is a unitary $(2|M| \times 2|M|)$-matrix, we have

$$\frac{\delta}{\delta \underline{b}} = \overline{U}\frac{\delta}{\delta \underline{a}}$$

and for any $\mu \in \mathcal{G}_M$

$$\prod_{\alpha \in M}\left(\frac{\delta}{\delta\overline{\psi}_\alpha}\frac{\delta}{\delta\psi_\alpha}\right)\mu\left(\overline{\psi},\psi\right) = \prod_{\alpha\in M}\left(\frac{\delta}{\delta\overline{\chi}_\alpha}\frac{\delta}{\delta\chi_\alpha}\right)\mu\left(\overline{\chi},\chi\right).$$

Proof. First we prove $\frac{\delta}{\delta\underline{b}} = \overline{U}\frac{\delta}{\delta\underline{a}}$. The identity $\frac{\delta}{\delta a_j}a_i = \delta_{ij}$ follows from the properties of the generators. An equivalent identity has to be claimed for $\frac{\delta}{\delta\underline{b}}\underline{b}$. Suppose $\frac{\delta}{\delta\underline{b}}$ transforms as $\frac{\delta}{\delta\underline{b}} = V\frac{\delta}{\delta\underline{a}}$ with a $(2|M| \times 2|M|)$-matrix V. This yields

$$\frac{\delta}{\delta b_j}b_i = \left(\sum_{\alpha\in\widetilde{M}} V_{j\alpha}\frac{\delta}{\delta a_\alpha}\right)\left(\sum_{\beta\in\widetilde{M}} U_{i\beta}a_\beta\right) = \left(UV^T\right)_{ij}.$$

In other words, we have to claim $UV^T = \mathbb{1}_{\widetilde{M}}$ and, thus, $V = \overline{U}$. Finally we can prove the invariance of the Grassmann integral. For a given set of generators $\{\overline{\psi}_i, \psi_i\}_{i\in M}$ any $\mu \in \mathcal{G}_M$ can be written as

$$\mu \equiv \mu\left(\overline{\psi},\psi\right) = \sum_{I,J\subseteq M}\alpha_{IJ}\overline{\Psi}_I\Psi_J$$

where the sum is over all ordered subsets I, J of M and $\alpha_{IJ} \in \mathbb{C}$ for all ordered subsets $I, J \subseteq M$. The Grassmann integral of μ is

$$\int \mathrm{d}(\overline{\Psi},\Psi)\,\mu\left(\overline{\psi},\psi\right) = \int \mathrm{d}\left(\overline{\Psi},\Psi\right)\sum_{I,J\subseteq M} a_{IJ}\overline{\Psi}_I\Psi_J = \int \mathrm{d}\left(\overline{\Psi},\Psi\right)\,\alpha_{MM}\overline{\Psi}_M\Psi_M$$

since all other terms of μ do not contribute to the integral. If the decomposition of μ yields $\alpha_{MM} = 0$, the Grassmann integral of μ vanishes. In this case the assertion is immediate. For $\alpha_{MM} \neq 0$ we consider the transformation of $\int \mathrm{d}(\overline{\Psi},\Psi)$ and $\overline{\Psi}_M\Psi_M$ separately. For $\int \mathrm{d}(\overline{\Psi},\Psi)$ we use

$\frac{\delta}{\delta \underline{a}_i}\frac{\delta}{\delta \underline{a}_j} = -\frac{\delta}{\delta \underline{a}_j}\frac{\delta}{\delta \underline{a}_i}$ for $i \neq j$ and express $\frac{\delta}{\delta \underline{b}}$ in terms of $\frac{\delta}{\delta \underline{a}}$:

$$\begin{aligned}\left(\prod_{\alpha\in M}\frac{\delta}{\delta\overline{\chi}_\alpha}\right)\left(\prod_{\alpha\in M}\frac{\delta}{\delta\chi_\alpha}\right) &= \prod_{\beta\in\widetilde{M}}\frac{\delta}{\delta\underline{b}_\beta}\\ &= \sum_{\beta_1,\ldots,\beta_{|\widetilde{M}|}\in\widetilde{M}}\prod_{j\in\widetilde{M}}\overline{U}_{j\beta_j}\frac{\delta}{\delta\underline{a}_{\beta_j}}\\ &= \sum_{\pi\in\mathcal{S}_{\widetilde{M}}}\prod_{j\in\widetilde{M}}\overline{U}_{j\pi(j)}\frac{\delta}{\delta\underline{a}_{\pi(j)}}\\ &= \sum_{\pi\in\mathcal{S}_{\widetilde{M}}}(-1)^\pi\prod_{j\in\widetilde{M}}\overline{U}_{j\pi(j)}\frac{\delta}{\delta\underline{a}_j}\\ &= \det\left(\overline{U}\right)\prod_{j\in\widetilde{M}}\frac{\delta}{\delta\underline{a}_j}.\end{aligned}$$

Analogously we have

$$\prod_{\alpha\in M}\overline{\chi}_M\prod_{\alpha\in M}\chi_M = \prod_{\beta\in\widetilde{M}}b_\beta = \det\left(U\right)\prod_{j\in\widetilde{M}}a_j.$$

Merging the results, we obtain

$$\left(\prod_{\alpha\in M}\frac{\delta}{\delta\overline{\chi}_\alpha}\right)\left(\prod_{\alpha\in M}\frac{\delta}{\delta\chi_\alpha}\right)\prod_{\alpha\in M}\overline{\chi}_M\prod_{\alpha\in M}\chi_M = \left|\det\left(U\right)\right|^2\prod_{j\in\widetilde{M}}\frac{\delta}{\delta\underline{a}_j}\prod_{j\in\widetilde{M}}a_j.$$

The proof is complete with $\left|\det\left(U\right)\right|^2 = 1$ which holds since U is unitary.□

Remark 5.14. The transformation U mixes $\overline{\psi}_i$'s and ψ_i's. For $U := \left(\begin{smallmatrix} u & v \\ \overline{v} & \overline{u}\end{smallmatrix}\right)$ a transformation without mixing is given for $v = 0$. In this case u has to be unitary.

For the application of the Grassmann integration on representability conditions we still need some tools, in particular the definition of a product on $\mathcal{G}_M$ which induces the CAR on the Grassmann algebra.

Definition 5.15. For all $\mu \equiv \mu\left(\overline{\psi},\psi\right)$ and $\eta \equiv \eta\left(\overline{\psi},\psi\right) \in \mathcal{G}_M$ we define the star product $\mu \star \eta \in \mathcal{G}_M$ by

$$\left(\mu\star\eta\right)\left(\overline{\psi},\psi\right) := \int \mathrm{d}(\overline{\Phi},\Phi)\,\mu\left(\overline{\psi},\phi\right)\eta\left(\overline{\phi},\psi\right)\mathrm{e}^{-\left(\overline{\Psi},\Psi\right)}\mathrm{e}^{\left(\overline{\Psi},\Phi\right)}\mathrm{e}^{-\left(\overline{\Phi},\Phi\right)}\mathrm{e}^{\left(\overline{\Phi},\Psi\right)}.$$

We calculate the star product of two monomials $\mu := \overline{\Psi}_I\Psi_J$ and $\eta := \overline{\Psi}_K\Psi_L$ for $I,J,K,L \subseteq M$ which determines the star product in general due to the linearity of the Grassmann integral.

Lemma 5.16. *Let $I,J,K,L \subseteq M$. Then we have*

$$\left(\overline{\Psi}_I\Psi_J\right)\star\left(\overline{\Psi}_K\Psi_L\right) = \sigma_S\sigma_{JS}\,\mathrm{e}^{-\left(\overline{\Psi},\Psi\right)}\overline{\Psi}_I\Psi_{J\setminus S}\overline{\Psi}_{K\setminus S}\Psi_L\prod_{\substack{\alpha\in M\\ \setminus(J\cup K)}}\left(1+\overline{\psi}_\alpha\psi_\alpha\right) \tag{5.10}$$

where $S := J \cap K$ *and* $\sigma_{JS} := (-1)^{|S|\left(|J\setminus S| + \frac{|S|-1}{2}\right)}$. σ_S *is given by the identity* $\sigma_S \Phi_S \Phi_{J\setminus S} \overline{\Phi}_S \overline{\Phi}_{K\setminus S} = \Phi_J \overline{\Phi}_K$.

Proof. Writing $S := J \cap K$ we face the integral

$$\left(\overline{\Psi}_I \Psi_J\right) \star \left(\overline{\Psi}_K \Psi_L\right) = \sigma_S \, \mathrm{e}^{-\left(\overline{\Psi},\Psi\right)} \overline{\Psi}_I \int \mathrm{d}(\overline{\Phi},\Phi)\, \Phi_S \Phi_{J\setminus S} \overline{\Phi}_S \overline{\Phi}_{K\setminus S} \times \prod_{\alpha\in M} \left(1 + \overline{\phi}_\alpha \psi_\alpha + \overline{\psi}_\alpha \phi_\alpha - \overline{\phi}_\alpha \phi_\alpha - \overline{\phi}_\alpha \phi_\alpha \overline{\psi}_\alpha \psi_\alpha\right) \Psi_L$$

where we use

$$\prod_{\alpha\in M} \left(1 + \overline{\phi}_\alpha \psi_\alpha + \overline{\psi}_\alpha \phi_\alpha - \overline{\phi}_\alpha \phi_\alpha - \overline{\phi}_\alpha \phi_\alpha \overline{\psi}_\alpha \psi_\alpha\right) = \mathrm{e}^{\left(\overline{\Psi},\Phi\right)} \mathrm{e}^{-\left(\overline{\Phi},\Phi\right)} \mathrm{e}^{\left(\overline{\Phi},\Psi\right)}$$

as a consequence of (5.8). In the next step we write

$$M = (M \setminus (J \cup K)) \,\dot\cup\, (J \setminus S) \,\dot\cup\, (K \setminus S) \,\dot\cup S$$

(where $\dot\cup$ denotes a disjoint union) and arrive at

$$\begin{aligned}\left(\overline{\Psi}_I \Psi_J\right) \star \left(\overline{\Psi}_K \Psi_L\right) =& \sigma_S \sigma_{SJ} \, \mathrm{e}^{-\left(\overline{\Psi},\Psi\right)} \overline{\Psi}_I \int \mathrm{d}(\overline{\Phi},\Phi) \prod_{\alpha\in S} \phi_\alpha \overline{\phi}_\alpha \\ &\times \prod_{\alpha\in J\setminus S} \left(\phi_\alpha + \phi_\alpha \overline{\phi}_\alpha \psi_\alpha\right) \prod_{\alpha\in K\setminus S} \left(\overline{\phi}_\alpha + \overline{\phi}_\alpha \overline{\psi}_\alpha \phi_\alpha\right) \\ &\times \prod_{\substack{\alpha\in M\\ \setminus(J\cup K)}} \left(1 + \overline{\phi}_\alpha \psi_\alpha + \overline{\psi}_\alpha \phi_\alpha - \overline{\phi}_\alpha \phi_\alpha - \overline{\phi}_\alpha \phi_\alpha \overline{\psi}_\alpha \psi_\alpha\right) \Psi_L .\end{aligned}$$

The sign $\sigma_{JS} := (-1)^{|S|\left(|J\setminus S| + \frac{|S|-1}{2}\right)}$ occurs due to the permutation of all ϕ's in Φ_S with all ϕ's in $\Phi_{J\setminus S}$, and $\Phi_S \overline{\Phi}_S = (-1)^{\frac{1}{2}|S|(|S|-1)} \left(\prod_{\alpha\in S} \phi_\alpha \overline{\phi}_\alpha\right)$. Now we can perform the integration and arrive at

$$\begin{aligned}&\left(\overline{\Psi}_I \Psi_J\right) \star \left(\overline{\Psi}_K \Psi_L\right) \\ &= \sigma_S \sigma_{JS} \, \mathrm{e}^{-\left(\overline{\Psi},\Psi\right)} \overline{\Psi}_I \prod_{\alpha\in J\setminus S} \psi_\alpha \prod_{\alpha\in K\setminus S} \overline{\psi}_\alpha \prod_{\substack{\alpha\in M\\ \setminus(J\cup K)}} \left(1 + \overline{\psi}_\alpha \psi_\alpha\right) \Psi_L\end{aligned}$$

as claimed in (5.10) since all involved sets are disjoint. □

There are several properties of the star product which follow from Lemma 5.16.

Lemma 5.17. *For all* $\mu, \eta, \nu \in \mathcal{G}_M$ *we have*

$$\mu \star (\eta \star \nu) = (\mu \star \eta) \star \nu .$$

Proof. By the definition of the star product we have

$$\begin{aligned}\mu \star (\eta \star \nu) &= \mu\left(\overline{\psi},\psi\right) \star \int \mathrm{d}(\overline{\Phi},\Phi)\, \eta\left(\overline{\psi},\phi\right) \nu\left(\overline{\phi},\psi\right) \\ &\qquad \times \mathrm{e}^{-\left(\overline{\Psi},\Psi\right)+\left(\overline{\Psi},\Phi\right)-\left(\overline{\Phi},\Phi\right)+\left(\overline{\Phi},\Psi\right)} \\ &= \int \mathrm{d}(\overline{\Xi},\Xi) \int \mathrm{d}(\overline{\Phi},\Phi)\, \mu\left(\overline{\psi},\xi\right) \eta\left(\overline{\xi},\phi\right) \nu\left(\overline{\phi},\psi\right) \\ &\qquad \times \mathrm{e}^{-\left(\overline{\Psi},\Psi\right)+\left(\overline{\Psi},\Xi\right)-\left(\overline{\Xi},\Xi\right)+\left(\overline{\Xi},\Phi\right)-\left(\overline{\Phi},\Phi\right)+\left(\overline{\Phi},\Psi\right)} .\end{aligned}$$

Performing the integration with respect to $(\overline{\phi}, \phi)$, we gain

$$\mu \star (\eta \star \nu) = \int \mathrm{d}(\overline{\Xi}, \Xi)\, \mu\left(\overline{\psi}, \xi\right) \eta\left(\overline{\xi}, \psi\right) \mathrm{e}^{-(\overline{\Psi}\Psi)+(\overline{\Psi},\Xi)-(\overline{\Xi},\Xi)+(\overline{\Xi},\Psi)} \star \nu\left(\overline{\psi}, \psi\right)$$

which is actually $(\mu \star \eta) \star \nu$. □

As for the creation and annihilation operators on $\mathcal{B}(\wedge\mathcal{H})$ there is also an implementation of the CAR for the generators of $\mathcal{G}_M$.

Lemma 5.18. *Let $\{\overline{\psi}_i, \psi_i\}_{i\in M}$ be the generators of $\mathcal{G}_M$. With $\{\mu, \eta\}_\star := \mu \star \eta + \eta \star \mu$ we have*

$$\{\psi_i, \psi_j\}_\star = \left\{\overline{\psi}_i, \overline{\psi}_j\right\}_\star = 0, \qquad \text{and} \qquad \{\overline{\psi}_i, \psi_j\}_\star = \delta_{ij}$$

for any $i, j \in M$.

Proof. The identities follow directly from Lemma 5.16 by an appropriate choice of I, J, K, and L. We observe that

$$\mathrm{e}^{-(\overline{\Psi},\Psi)} \prod_{\substack{\alpha\in M\\ \setminus(J\cup K)}} \left(1 + \overline{\psi}_\alpha \psi_\alpha\right) = \prod_{\alpha\in J\cup K} \left(1 - \overline{\psi}_\alpha \psi_\alpha\right)$$

and conclude for the first identity with $I = K = \emptyset$, $J = \{i\}$, and $L = \{j\}$ in (5.10) that $S = \emptyset$ and therefore $\sigma_S = \sigma_{JS} = 1$. This yields

$$\psi_i \star \psi_j = \left(1 - \overline{\psi}_i \psi_i\right) \psi_i \psi_j = \psi_i \psi_j. \tag{5.11}$$

Setting $J = \{j\}$ and $L = \{i\}$ we gain $\psi_j \star \psi_i = \psi_j \psi_i$ and hence $\psi_i \star \psi_j + \psi_j \star \psi_i = \psi_i \psi_j + \psi_j \psi_i = 0$. Equivalently we obtain $\overline{\psi}_i \overline{\psi}_j + \overline{\psi}_j \overline{\psi}_i = 0$.
For the last identity we set $J = K = \emptyset$, $I = \{i\}$, and $L = \{j\}$. On the one hand, (5.10) leads to

$$\overline{\psi}_i \star \psi_j = \overline{\psi}_i \psi_j$$

which is valid for both $i = j$ and $i \neq j$. On the other hand, with $I = L = \emptyset$, $J = \{j\}$, and $K = \{i\}$ we have to distinguish between the cases $J = K$ and $J \neq K$. For $J \neq K$ we have

$$\psi_j \star \overline{\psi}_i = \left(1 - \overline{\psi}_i \psi_i\right) \left(1 - \overline{\psi}_j \psi_j\right) \psi_j \overline{\psi}_i = \psi_j \overline{\psi}_i.$$

For $J = K$ we have $S = J = K$ and thus

$$\psi_j \star \overline{\psi}_i = \left(1 - \overline{\psi}_i \psi_i\right). \tag{5.12}$$

The last two results together give $\psi_j \star \overline{\psi}_i = \delta_{ij} - \overline{\psi}_i \psi_j$. Finally we arrive at $\overline{\psi}_i \star \psi_j + \psi_j \star \overline{\psi}_i = \delta_{ij}$. We mention that in (5.11)-(5.12) $\sigma_S = \sigma_{JS} = 1$ due to the choice of the sets I, J, K, and L. □

By a straightforward calculation using Lemma 5.16 one can also show that for any generator $\{\overline{\psi}_i, \psi_i\}_{i\in M}$ of $\mathcal{G}_M$ we have the following:

Corollary 5.19. *Let $\{\overline{\psi}_i, \psi_i\}_{i\in M}$ be the generators of $\mathcal{G}_M$. Then we have*

$$\overline{\psi}_{i_1} \star \cdots \star \overline{\psi}_{i_m} \star \psi_{j_1} \star \cdots \star \psi_{j_n} = \overline{\psi}_{i_1} \cdots \overline{\psi}_{i_m} \psi_{j_1} \cdots \psi_{j_n}.$$

Proof. We use the associativity $\left(\overline{\psi}_{i_1} \star \cdots \star \overline{\psi}_{i_m}\right) \star (\psi_{j_1} \star \cdots \star \psi_{j_n}) = \overline{\psi}_{i_1} \star \cdots \star \overline{\psi}_{i_m} \star \psi_{j_1} \star \cdots \star \psi_{j_n}$ and calculate the brackets using Lemma 5.16. For the first bracket we set in (5.10) $I = \{i_1, \ldots, i_m\}$ and $J = K = L = \emptyset$. For the second bracket we use $I = J = K = \emptyset$ and $L = \{j_1, \ldots, j_n\}$. For both we have $\sigma_S = \sigma_{JS} = 1$ and conclude

$$\overline{\psi}_{i_1} \star \cdots \star \overline{\psi}_{i_m} \star \psi_{j_1} \star \cdots \star \psi_{j_n} = \left(\overline{\psi}_{i_1} \cdots \overline{\psi}_{i_m}\right) \star (\psi_{j_1} \cdots \psi_{j_n}).$$

The last star product can be calculated by setting $I = \{i_1, \ldots, i_m\}$, $L = \{j_1, \ldots, j_n\}$, and $J = K = \emptyset$ in (5.10). Again, $\sigma_S = \sigma_{JS} = 1$, and we arrive at the assertion. □

We emphasize that

$$\overline{\psi}_i \psi_j = \overline{\psi}_i \star \psi_j, \quad \text{but} \quad \psi_i \overline{\psi}_j = -\overline{\psi}_j \psi_i = -\overline{\psi}_j \star \psi_i.$$

This implies that the star product can be inserted (or skipped) only if the monomial in ψ and $\overline{\psi}$ is normal-ordered (i.e., all $\overline{\psi}$'s are to the left of all ψ's). As follows from the proof, monomials containing only ψ's or $\overline{\psi}$'s can also be considered as normal-ordered in the sense that we can identify $\overline{\psi}_{i_1} \star \cdots \star \overline{\psi}_{i_m} = \overline{\psi}_{i_1} \cdots \overline{\psi}_{i_m}$ and $\psi_{j_1} \star \cdots \star \psi_{j_n} = \psi_{j_1} \cdots \psi_{j_n}$.

Lemma 5.20. *Let $N \in \mathbb{N}$ and $A_i \in \mathcal{B}(\wedge\mathcal{H})$ for $i \in \{1, \ldots, N\}$. Then*

$$\Theta(A_1 A_2 \cdots A_N) = \Theta(A_1) \star \Theta(A_2) \star \cdots \star \Theta(A_N). \tag{5.13}$$

Proof. Due to the associativity of the star product it suffices to consider the assertion for $N = 2$. We use the CAR to establish normal order in the product $A_1 A_2 \in \mathcal{B}(\wedge\mathcal{H})$ and indicate this order by $\vdots A_1 A_2 \vdots$. For some $a_{\substack{i_1 \ldots i_m \\ j_1 \ldots j_n}} \in \mathbb{C}$ we can write

$$\vdots A_1 A_2 \vdots = \sum_{m,n} \sum_{\substack{i_1 \ldots i_m \\ j_1 \ldots j_n} \in M} a_{\substack{i_1 \ldots i_m \\ j_1 \ldots j_n}} c^*_{i_1} \cdots c^*_{i_m} c_{j_1} \cdots c_{j_n}$$

and apply Θ. Using Corollary 5.19 we arrive at

$$\Theta(\vdots A_1 A_2 \vdots) = \sum_{m,n} \sum_{\substack{i_1 \ldots i_m \\ j_1 \ldots j_n} \in M} a_{\substack{i_1 \ldots i_m \\ j_1 \ldots j_n}} \overline{\psi}_{i_1} \star \cdots \star \overline{\psi}_{i_m} \star \psi_{j_1} \star \cdots \star \psi_{j_m}. \tag{5.14}$$

Now we can use the CAR on $\mathcal{G}_M$ to restore the same order we had in $A_1 A_2$ within the r.h.s. of (5.14) and recognize that it equals $\Theta(A_1) \star \Theta(A_2)$. In other words we have

$$\sum_{m,n} \sum_{\substack{i_1 \ldots i_m \\ j_1 \ldots j_n} \in M} a_{\substack{i_1 \ldots i_m \\ j_1 \ldots j_n}} \overline{\psi}_{i_1} \star \cdots \star \overline{\psi}_{i_m} \star \psi_{j_1} \star \cdots \star \psi_{j_m} = \vdots \Theta(A_1) \star \Theta(A_2) \vdots,$$

which gives the assertion. □

We can equip $(\mathcal{G}_M, +, \star)$ with an involution $(\cdot)^*$ such that $(\mathcal{G}_M, +, \star, ^*)$ becomes a *-algebra.

Definition 5.21. For all $\mu_i \in \mathcal{G}_M$ with $i \in \mathbb{N}$ and $c \in \mathbb{C}$ the involution $(\cdot)^*$ on $(\mathcal{G}_M, +, \star)$ is defined by $(\psi_i)^* := \overline{\psi}_i$ and $(\overline{\psi}_i)^* := \psi_i$ for any $i \in M$, and

$$(c\,\mu_1 \cdots \mu_n)^* := \bar{c}\,\mu_n^* \cdots \mu_1^* .$$

Remark 5.22. For $\mu \equiv \mu\left(\overline{\psi}, \phi\right) := \sum_{I,J} a_{IJ}\, \overline{\Psi}_I \Phi_J$ and $a_{IJ} \in \mathbb{C}$ the involution μ^* is $\mu^*\left(\overline{\phi}, \psi\right) = \sum_{I,J} \bar{a}_{IJ}\, \overline{\Phi}_{J'} \Psi_{I'} = \sum_{I,J} (-1)^{\frac{1}{2}|I|(|I|-1)+\frac{1}{2}|J|(|J|-1)}\, \bar{\alpha}_{IJ}\, \overline{\Phi}_J \Psi_I$. We emphasize that $\left(\mu\left(\overline{\psi}, \phi\right)\right)^* = \mu^*\left(\overline{\phi}, \psi\right) \neq \left(\mu\left(\overline{\phi}, \psi\right)\right)^*$.

Lemma 5.23. *The involution in Definition 5.21 is compatible with Θ, the Grassmann integration, and the star product:*

a) $\Theta\left((\cdot)^*\right) = \left(\Theta\left(\cdot\right)\right)^*$,

b) $\int \mathrm{d}(\overline{\Psi}, \Psi)\,(\cdot)^* = \left[\int \mathrm{d}(\overline{\Psi}, \Psi)\,(\cdot)\right]^*$,

c) $(\mu \star \eta)^* = \eta^* \star \mu^*$.

Proof. We prove *a*) and *b*). *c*) is a consequence of *b*).

a) For any $I, J \subseteq M$ we abbreviate $C_I^* := c_{i_1}^* \cdots c_{i_m}^*$ and $C_J := c_{j_1} \cdots c_{j_n}$ and write any $A \in \mathcal{B}(\mathcal{H})$ as $A = \sum_{I,J} a_{IJ}\, C_I^* C_J$ for some $a_{IJ} \in \mathbb{C}$. This leads to

$$\begin{aligned}(\Theta\left(A\right))^* &= \Big(\sum_{I,J} a_{IJ}\, \overline{\Psi}_I \Psi_J\Big)^* = \sum_{I,J} \bar{a}_{IJ}\, \overline{\Psi}_{J'} \Psi_{I'} = \Theta\Big(\sum_{I,J} \bar{a}_{IJ}\, C_{J'}^* C_{I'}\Big) \\ &= \Theta\Big(\Big(\sum_{I,J} a_{IJ}\, C_I^* C_J\Big)^*\Big) = \Theta\left(A^*\right).\end{aligned}$$

b) For a fixed, but arbitrary $i \in M$ and $\mu \in \mathcal{G}_M$ we formally have $\left(\frac{\delta}{\delta\overline{\psi}_i}\frac{\delta}{\delta\psi_i}\right)^* \mu = \frac{\delta}{\delta\overline{\psi}_i}\frac{\delta}{\delta\psi_i}\mu$ which gives the assertion.

c) We calculate the l.h.s. of *c*) using *b*) and Remark 5.22:

$$\begin{aligned}(\mu \star \eta)^* &= \int \mathrm{d}(\overline{\Phi}, \Phi)\, \eta^*\left(\overline{\psi}, \phi\right) \mu^*\left(\overline{\phi}, \psi\right) \mathrm{e}^{-(\overline{\Psi}, \Psi)} \mathrm{e}^{(\overline{\Psi}, \Phi)} \mathrm{e}^{-(\overline{\Phi}, \Phi)} \mathrm{e}^{(\overline{\Phi}, \Psi)} \\ &= \eta^* \star \mu^*\end{aligned}$$

since $\left(\mathrm{e}^{(\cdot)}\right)^* = \mathrm{e}^{(\cdot)}$. □

A key property of the Grassmann integral for deriving representability conditions as in the next section is the cyclicity property which has its equivalent in the cyclicity of the trace, i.e., $\mathrm{tr}_{\wedge\mathcal{H}}\left(AB\right) = \mathrm{tr}_{\wedge\mathcal{H}}\left(BA\right)$.

Theorem 5.24. *For $\mu, \eta \in \mathcal{G}_M$ we have*

$$\int \mathcal{D}(\overline{\Psi}, \Psi)\,(\mu \star \eta) = \int \mathcal{D}(\overline{\Psi}, \Psi)\,(\eta \star \mu).$$

Proof. Without loss of generality we can set

$$\mu := \overline{\Psi}_I \Psi_J \quad \text{and} \quad \eta := \overline{\Psi}_K \Psi_L$$

and observe with (5.10) and $T := I \cap L$

$$\int \mathcal{D}(\overline{\Psi}, \Psi)\, \mu \star \eta = \sigma_S \sigma_T \sigma_{JS} \int \mathcal{D}(\overline{\Psi}, \Psi) \cdot \mathrm{e}^{-(\overline{\Psi}, \Psi)} \\ \times \overline{\Psi}_T \overline{\Psi}_{I\setminus T} \prod_{\alpha \in J\setminus S} \psi_\alpha \prod_{\alpha \in K\setminus S} \overline{\psi}_\alpha \prod_{\substack{\alpha \in M \\ \setminus (J\cup K)}} (1 + \overline{\psi}_\alpha \psi_\alpha)\, \Psi_T \Psi_{L\setminus T}.$$

Afterwards, we rearrange the factors and arrive at

$$\int \mathcal{D}(\overline{\Psi}, \Psi)\, \mu \star \eta = \sigma_S \sigma_T \tilde{\sigma} \int \mathrm{d}(\overline{\Psi}, \Psi)\, \overline{\Psi}_{I\setminus T} \overline{\Psi}_{K\setminus S} \Psi_{J\setminus S} \Psi_{L\setminus T} \prod_{\alpha \in T} \overline{\psi}_\alpha \psi_\alpha \\ \times \prod_{\alpha \in M} (1 + \overline{\psi}_\alpha \psi_\alpha) \prod_{\substack{\alpha \in M \\ \setminus (J\cup K)}} (1 + \overline{\psi}_\alpha \psi_\alpha) \tag{5.15}$$

where $\tilde{\sigma} \in \{\pm 1\}$ corresponds to the signs resulting from the anticommutations and is

$$\tilde{\sigma} := (-1)^{|S||J\setminus S| + |T||K\setminus S| + \frac{1}{2}|S|(|S|-1) + \frac{1}{2}|T|(|T|-1) + |T||J\setminus S| + |T||I\setminus T| + |K\setminus S||J\setminus S|}.$$

In order to go on, we need some preparation. First of all we observe that

$$\prod_{\alpha \in M} (1 + \overline{\psi}_\alpha \psi_\alpha) \prod_{\substack{\alpha \in M \\ \setminus (J\cup K)}} (1 + \overline{\psi}_\alpha \psi_\alpha) \\ = \prod_{\substack{\alpha \in M \\ \setminus (J\cup K)}} (1 + 2\overline{\psi}_\alpha \psi_\alpha) \prod_{\alpha \in J\cup K} (1 + \overline{\psi}_\alpha \psi_\alpha).$$

On the one hand, we have $J \cup K = (J \setminus S) \,\dot\cup\, (K \setminus S) \,\dot\cup S$ which implies

$$\prod_{\alpha \in J\cup K} (1 + \overline{\psi}_\alpha \psi_\alpha)\, \overline{\Psi}_{K\setminus S} \Psi_{J\setminus S} = \prod_{\alpha \in S} (1 + \overline{\psi}_\alpha \psi_\alpha)\, \overline{\Psi}_{K\setminus S} \Psi_{J\setminus S}.$$

On the other hand, we have by the same arguments

$$\prod_{\substack{\alpha \in M \\ \setminus (J\cup K)}} (1 + 2\overline{\psi}_\alpha \psi_\alpha)\, \overline{\Psi}_{I\setminus T} \overline{\Psi}_{K\setminus S} \Psi_{J\setminus S} \Psi_{L\setminus T} \prod_{\alpha \in T} \overline{\psi}_\alpha \psi_\alpha \\ = \prod_{\substack{\alpha \in M \\ \setminus (J\cup K\cup I\cup L)}} (1 + 2\overline{\psi}_\alpha \psi_\alpha)\, \overline{\Psi}_{I\setminus T} \overline{\Psi}_{K\setminus S} \Psi_{J\setminus S} \Psi_{L\setminus T} \prod_{\alpha \in T} \overline{\psi}_\alpha \psi_\alpha$$

since $I \cup L \equiv (I \setminus T) \,\dot\cup\, (L \setminus T) \,\dot\cup T$. Consequently our latter calculations lead in (5.15) to

$$\int \mathcal{D}(\overline{\Psi}, \Psi)\, \mu \star \eta = \sigma_S \sigma_T \tilde{\sigma} \int \mathrm{d}(\overline{\Psi}, \Psi)\, \overline{\Psi}_{I\setminus T} \overline{\Psi}_{K\setminus S} \Psi_{J\setminus S} \Psi_{L\setminus T} \prod_{\alpha \in T} \overline{\psi}_\alpha \psi_\alpha \\ \times \prod_{\alpha \in S} (1 + \overline{\psi}_\alpha \psi_\alpha) \prod_{\substack{\alpha \in M \\ \setminus (J\cup K\cup I\cup L)}} (1 + 2\overline{\psi}_\alpha \psi_\alpha). \tag{5.16}$$

Let us take a closer look at the involved sets. First of all we observe

(I) $K \setminus S \cap J \setminus S = \emptyset$

(II) $I \cup (K \setminus S) = L \cup (J \setminus S)$

(III) $I \cap (K \setminus S) = \emptyset$

(IV) $L \cap (J \setminus S) = \emptyset$.

In any other case we have $\int \mathcal{D}(\overline{\Psi}, \Psi)\, \mu \star \eta = \int \mathcal{D}(\overline{\Psi}, \Psi)\, \eta \star \mu = 0$. These observations have some consequences:

a) (II) and (I) $\Rightarrow$ $(K \setminus S) \subseteq L$ and $(J \setminus S) \subseteq I$ $\Rightarrow$ $\exists\ T_1, T_2 \subseteq M$ s.th. $I = (J \setminus S)\, \dot\cup T_1$ and $L = (K \setminus S)\, \dot\cup T_2$.

b) (III) and $I = (J \setminus S)\, \dot\cup T_1 \Rightarrow ((J \setminus S)\, \dot\cup T_1) \cap (K \setminus S) = \emptyset \Rightarrow T_1 \cap K \setminus S = \emptyset$. Analogously: (IV) and $L = (K \setminus S)\, \dot\cup T_1 \Rightarrow T_2 \cap (J \setminus S) = \emptyset$.

c) (II) and b) $\Rightarrow T_1 = T_2$, since all sets on the l.h.s. and r.h.s. of (II) are disjoint, respectively.

d) a), b) and c) $\Rightarrow L \cap I = ((K \setminus S)\, \dot\cup T_1) \cap ((J \setminus S)\, \dot\cup T_2) = T_1 \cap T_2 =: T$.

Back to a) we see that $I = (J \setminus S)\, \dot\cup T$ or $I \setminus T = J \setminus S$, and that $L = (K \setminus S)\, \dot\cup T$ implies $L \setminus T = K \setminus S$. This is illustrated in Figure 5.1.

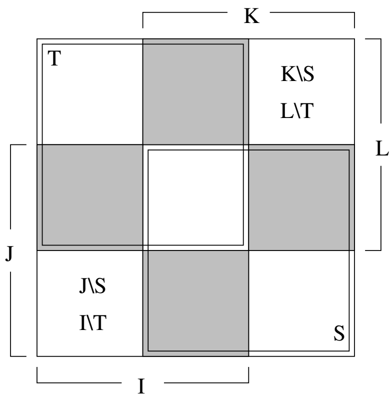

Figure 5.1: Breteaux chequerboard: *The integrals vanish if $J \cup L \neq I \cup K$. $S := J \cap K$ and $T := I \cap L$. Grey areas represent empty subsets.*

We come back to (5.16) and take the intersection $S \cap T$ into account. The term $\prod_{\alpha \in T} \overline{\psi}_\alpha \psi_\alpha \prod_{\alpha \in S} \left(1 + \overline{\psi}_\alpha \psi_\alpha\right)$ contributes to the integral as follows:

$$\prod_{\alpha \in T \cup S} \frac{\delta}{\delta \overline{\psi}_\alpha} \frac{\delta}{\delta \psi_\alpha} \prod_{\alpha \in T} \overline{\psi}_\alpha \psi_\alpha \prod_{\beta \in S} \left(1 + \overline{\psi}_\beta \psi_\beta\right) = \prod_{\alpha \in T \cup S} \frac{\delta}{\delta \overline{\psi}_\alpha} \frac{\delta}{\delta \psi_\alpha} \prod_{\alpha \in T \cup S} \overline{\psi}_\alpha \psi_\alpha$$

since $\prod_{\alpha\in T\cap S}\overline{\psi}_\alpha\psi_\alpha\prod_{\beta\in T\cap S}\left(1+\overline{\psi}_\beta\psi_\beta\right)=\prod_{\alpha\in T\cap S}\overline{\psi}_\alpha\psi_\alpha$ and

$$\begin{aligned}\prod_{\alpha\in S\setminus(T\cap S)}\frac{\delta}{\delta\overline{\psi}_\alpha}\frac{\delta}{\delta\psi_\alpha}\prod_{\beta\in S\setminus(T\cap S)}&\left(1+\overline{\psi}_\beta\psi_\beta\right)\\&=\prod_{\alpha\in S\setminus(T\cap S)}\frac{\delta}{\delta\overline{\psi}_\alpha}\frac{\delta}{\delta\psi_\alpha}\prod_{\beta\in S\setminus(T\cap S)}\overline{\psi}_\beta\psi_\beta.\end{aligned}$$

This finishes our calculations and we conclude:

$$\begin{aligned}\int\mathcal{D}(\overline{\Psi},\Psi)\,\mu\star\eta=\sigma_S\sigma_T\tilde{\sigma}\int\mathrm{d}(\overline{\Psi},\Psi)&\prod_{\alpha\in T\cup S}\overline{\psi}_\alpha\psi_\alpha\\\times&\prod_{\substack{\alpha\in M\\\setminus(J\cup K\cup I\cup L)}}\left(1+2\overline{\psi}_\alpha\psi_\alpha\right)\overline{\Psi}_{I\setminus T}\overline{\Psi}_{K\setminus S}\Psi_{J\setminus S}\Psi_{L\setminus T}.\end{aligned}\tag{5.17}$$

The r.h.s. of the assertion in Theorem 5.24 can be calculated analogously. The result is

$$\begin{aligned}\int\mathcal{D}(\overline{\Psi},\Psi)\,\eta\star\mu=\sigma_T\sigma_S\widehat{\sigma}\int\mathrm{d}(\overline{\Psi},\Psi)&\prod_{\alpha\in S\cup T}\overline{\psi}_\alpha\psi_\alpha\\\times&\prod_{\substack{\alpha\in M\\\setminus(J\cup K\cup I\cup L)}}\left(1+2\overline{\psi}_\alpha\psi_\alpha\right)\overline{\Psi}_{K\setminus S}\overline{\Psi}_{I\setminus T}\Psi_{L\setminus T}\Psi_{J\setminus S}\end{aligned}$$

where the sign resulting from the anticommutations is

$$\widehat{\sigma}:=(-1)^{|T||L\setminus T|+|S||L\setminus T|+\frac{1}{2}|S|(|S|-1)+\frac{1}{2}|T|(|T|-1)+|S||I\setminus T|+|S||K\setminus S|+|I\setminus T||L\setminus T|}.$$

The l.h.s. and the r.h.s. of Theorem 5.24 are symmetric with respect to the involved sets. The proof is complete by the observation

$$\tilde{\sigma}=\widehat{\sigma}=(-1)^{\frac{1}{2}|S|(|S|-1)+\frac{1}{2}|T|(|T|-1)+|K\setminus S||J\setminus S|+|T||K\setminus S|+|S||J\setminus S|}$$

which follows from $I\setminus T=J\setminus S$ and $L\setminus T=K\setminus S$. □

Remark 5.25. The integral on the r.h.s. of (5.17) can be carried out. Abbreviating $s_Q:=\frac{1}{2}|Q|\,(|Q|-1)$ for $Q\subseteq M$, we have

$$\begin{aligned}\int\mathcal{D}(\overline{\Psi},\Psi)\,\mu\star\eta&=\sigma_S\sigma_T\,(-1)^{s_S+s_T+|T||K\setminus S|+|S||J\setminus S|+s_{I\setminus T}+s_{K\setminus S}}\\&\quad\times\int\mathrm{d}(\overline{\Psi},\Psi)\prod_{\alpha\in I\setminus T}\overline{\psi}_\alpha\psi_\alpha\prod_{\alpha\in K\setminus S}\overline{\psi}_\alpha\psi_\alpha\prod_{\alpha\in T\cup S}\overline{\psi}_\alpha\psi_\alpha\\&\quad\times\prod_{\alpha\in M\setminus(I\cup K)}\left(1+2\overline{\psi}_\alpha\psi_\alpha\right)\\&=\sigma_S\sigma_T\,(-1)^{s_S+s_T+|T||K\setminus S|+|S||J\setminus S|+s_{I\setminus T}+s_{K\setminus S}}\\&\quad\times(-1)^{|I\setminus T|+|K\setminus S|+|T\cup S|}\,(-2)^{|M|-|I\cup K|}.\end{aligned}$$

With $|I\setminus T|+|K\setminus S|+|T\cup S|=|I\cup K|$ we obtain

$$\int\mathcal{D}(\overline{\Psi},\Psi)\,\mu\star\eta=\sigma_S\sigma_T\,(-1)^{s_J+s_L}\,2^{|M|-|I\cup K|}$$

for $\mu:=\overline{\Psi}_I\Psi_J$ and $\eta:=\overline{\Psi}_K\Psi_L$.

Remark 5.26. A consequence of Lemmas 5.17 and 5.24 is the invariance of the Grassmann integral with respect to cyclic permutations of the integrand:

$$\int \mathrm{d}(\overline{\Psi}, \Psi)\, (\mu_1 \star \mu_2 \star \cdots \star \mu_N) = \int \mathrm{d}(\overline{\Psi}, \Psi)\, (\mu_2 \star \cdots \star \mu_N \star \mu_1)\,. \tag{5.18}$$

This also holds true for $\int \mathcal{D}(\overline{\Psi}, \Psi)\, (\,\cdot\,)$ since $\mathrm{e}^{2(\overline{\Psi}, \Psi)}$ commutes with every Grassmann variable.

Given an involution on $(\mathcal{G}_M, +, \star)$, we define the property of non-negativity on $\mathcal{G}_M$ as follows.

Definition 5.27. We call $\mu \in \mathcal{G}_M$ positive semi-definite, shortly $\mu \geq 0$, if there exists an $\eta \in \mathcal{G}_M$ such that

$$\mu = \eta^* \star \eta.$$

Approaching the problem of representability by Grassmann integration, an important result is the following theorem.

Theorem 5.28. *For any $\mu \in \mathcal{G}_M$ with $\mu \geq 0$ we have*

$$(-1)^{|M|} \int \mathcal{D}(\overline{\Psi}, \Psi)\, \mu \geq 0. \tag{5.19}$$

Proof. We use an induction in $|M|$. For this purpose we write any $\xi \in \mathcal{G}_{M+1} := \mathrm{span}\left\{\overline{\psi}_1, \ldots, \overline{\psi}_{|M|}, \overline{\psi}_{|M|+1}, \psi_1, \ldots, \psi_{|M|}, \psi_{|M|+1}\right\}$ as

$$\xi = \eta_{00} + \eta_{01}\psi_{|M|+1} + \overline{\psi}_{|M|+1}\eta_{10} + \overline{\psi}_{|M|+1}\eta_{11}\psi_{|M|+1} \tag{5.20}$$

for normal-ordered $\eta_{00}, \eta_{01}, \eta_{10}, \eta_{11} \in \mathcal{G}_M$. We indicate integration with respect to a certain index set M by writing $\int \mathrm{d}_M(\overline{\Psi}, \Psi)$ and $\int \mathcal{D}_M(\overline{\Psi}, \Psi)$, respectively. Furthermore we recall that

$$\begin{aligned} \mathrm{e}^{E_M} &:= \mathrm{e}^{(\overline{\Psi}, \Psi)} \mathrm{e}^{(\overline{\Psi}, \Phi)} \mathrm{e}^{-(\overline{\Phi}, \Phi)} \mathrm{e}^{(\overline{\Phi}, \Psi)} \\ &= \prod_{\alpha=1}^{M} \left(1 - \overline{\phi}_\alpha \phi_\alpha + \overline{\psi}_\alpha \psi_\alpha + \overline{\phi}_\alpha \psi_\alpha + \overline{\psi}_\alpha \phi_\alpha - 2\overline{\psi}_\alpha \psi_\alpha \overline{\phi}_\alpha \phi_\alpha\right). \end{aligned}$$

In order to show (5.19) for $|M| = 0$, we consider $\mu := a^* \star a \in \mathcal{G}_0$ with $a \in \mathbb{C}$, and observe that with $\int \mathcal{D}_0(\overline{\Psi}, \Psi) = 1$ the l.h.s. of (5.19) is non-negative,

$$\int \mathcal{D}_0(\overline{\Psi}, \Psi)\, \mu = |a|^2 \geq 0.$$

Now we assume that (5.19) holds for $|M|$ and consider the l.h.s. of (5.19) for $|M|+1$ and $\mu = \xi^* \star \xi$. We abbreviate $\psi_{|M|+1} \equiv \psi'$ and $\overline{\psi}_{|M|+1} \equiv \overline{\psi'}$.

$$\begin{aligned}(-1)^{|M|+1} &\int \mathcal{D}_{M+1}(\overline{\Psi},\Psi)\,(\xi^* \star \xi) \\ &= (-1)^{|M|+1} \int \mathcal{D}_{M+1}(\overline{\Psi},\Psi)\Big[\eta_{00}^* \star \eta_{00} + \eta_{00}^* \star \left(\overline{\psi'}\,\eta_{11}\psi'\right) \\ &\qquad + \left(\overline{\psi'}\,\eta_{01}^*\right) \star (\eta_{01}\psi') + (\eta_{10}^*\psi') \star \left(\overline{\psi'}\,\eta_{10}\right) + \left(\overline{\psi'}\,\eta_{11}^*\psi'\right) \star \eta_{00} \\ &\qquad\qquad + \left(\overline{\psi'}\,\eta_{11}^*\psi'\right) \star \left(\overline{\psi'}\,\eta_{11}\psi'\right)\Big].\end{aligned} \tag{5.21}$$

Other terms like $\int \mathcal{D}_{M+1}(\overline{\Psi},\Psi)\eta_{00}^* \star (\eta_{01}\psi')$ vanish, as can be seen in (5.16) since in this case $I \cup K \neq J \cup L$.

In the next step we use $\int \mathrm{d}_{M+1}(\overline{\Psi},\Psi) = \int \mathrm{d}_M(\overline{\Psi},\Psi)\frac{\delta}{\delta\overline{\psi'}}\frac{\delta}{\delta\psi'}$ and the definition of the star product to carry out all integrations with respect to ψ' and $\overline{\psi'}$. We exemplify this step by the last term on the r.h.s. of (5.21):

$$\begin{aligned}(-1)^{|M|+1} &\int \mathcal{D}_{M+1}(\overline{\Psi},\Psi)\left(\overline{\psi'}\,\eta_{11}^*\psi'\right) \star \left(\overline{\psi'}\,\eta_{11}\psi'\right) \\ &= (-1)^{|M|+1} \int \mathrm{d}_{M+1}(\overline{\Psi},\Psi) \int \mathrm{d}_{M+1}\left(\overline{\Phi},\Phi\right) \overline{\psi'}\,\eta_{11}^*\left(\overline{\psi},\phi\right)\phi' \\ &\qquad\qquad \times \overline{\phi'}\,\eta_{11}\left(\overline{\phi},\psi\right)\psi'\,\mathrm{e}^{E_{M+1}}.\end{aligned}$$

Since $\eta_{11}^*\left(\overline{\psi},\phi\right)\eta_{11}\left(\overline{\phi},\psi\right)$ is even in the variables $\left(\overline{\psi},\psi,\overline{\phi},\phi\right)$, we continue with

$$\begin{aligned}(-1)^{|M|+1} &\int \mathcal{D}_{M+1}(\overline{\Psi},\Psi)\left(\overline{\psi'}\,\eta_{11}^*\psi'\right) \star \left(\overline{\psi'}\,\eta_{11}\psi'\right) \\ &= (-1)^{|M|+1} \int \mathrm{d}_M(\overline{\Psi},\Psi) \int \mathrm{d}_M\left(\overline{\Phi},\Phi\right)\eta_{11}^*\left(\overline{\psi},\phi\right)\eta_{11}\left(\overline{\phi},\psi\right)\mathrm{e}^{E_M} \\ &\times \frac{\delta}{\delta\overline{\phi'}}\frac{\delta}{\delta\phi'}\frac{\delta}{\delta\overline{\psi'}}\frac{\delta}{\delta\psi'}\overline{\psi'}\phi'\overline{\phi'}\psi'\left(1-\overline{\phi'}\phi'+\overline{\psi'}\psi'+\overline{\phi'}\psi'+\overline{\psi'}\phi'-2\overline{\psi'}\psi'\overline{\phi'}\phi'\right) \\ &= (-1)^{|M|+2} \int \mathcal{D}_M(\overline{\Psi},\Psi)\,\eta_{11}^* \star \eta_{11}.\end{aligned}$$

By analogous calculations we obtain

$$\begin{aligned}(-1)^{|M|+1} &\int \mathcal{D}_{M+1}(\overline{\Psi},\Psi)\,(\xi^* \star \xi) \\ &= (-1)^{|M|+2} \int \mathcal{D}_M(\overline{\Psi},\Psi)\Big[2\eta_{00}^* \star \eta_{00} + \eta_{00}^* \star \tilde{\eta}_{11} + \eta_{01}^* \star \eta_{01} + \eta_{10}^* \star \eta_{10} \\ &\qquad\qquad + \tilde{\eta}_{11}^* \star \eta_{00} + \eta_{11}^* \star \eta_{11}\Big]\end{aligned}$$

where $\tilde{\eta}_{11} := \sum_{I,J}(-1)^{|I|+|J|}a_{IJ}\overline{\Psi}_I\Psi_J \in \mathcal{G}_M$ if $\eta_{11} := \sum_{I,J}a_{IJ}\overline{\Psi}_I\Psi_J$ for some $a_{IJ} \in \mathbb{C}$. $\tilde{\eta}_{11}$ occurs due to the anticommutations of ψ_{M+1} with η_{11}^* and of $\overline{\psi}_{M+1}$ with η_{11} in the second and the fifth term on the r.h.s. of (5.21), respectively. Observing that

$$\begin{aligned}
&\int \mathcal{D}_M(\overline{\Psi},\Psi)\, \tilde{\eta}_{11}^* \star \tilde{\eta}_{11} \\
&\quad = \sum_{I,J,K,L} a_{IJ}\bar{a}_{LK}\, (-1)^{|I|+|J|+|K|+|L|} \int \mathcal{D}_M(\overline{\Psi},\Psi)\, \left(\overline{\Psi}_I \Psi_J\right) \star \left(\overline{\Psi}_K \Psi_L\right) \\
&\quad = \int \mathcal{D}_M(\overline{\Psi},\Psi)\, \eta_{11}^* \star \eta_{11}
\end{aligned}$$

since $|I|+|J|+|K|+|L|$ is even (otherwise both integrals vanish), we finally conclude

$$\begin{aligned}
&(-1)^{|M|+1} \int \mathcal{D}_{M+1}(\overline{\Psi},\Psi)\, (\xi^* \star \xi) \\
&\quad = (-1)^{|M|+2} \int \mathcal{D}_M(\overline{\Psi},\Psi) \Big[\eta_{00}^* \star \eta_{00} + (\eta_{00} + \tilde{\eta}_{11})^* \star (\eta_{00} + \tilde{\eta}_{11}) \\
&\qquad\qquad + \eta_{01}^* \star \eta_{01} + \eta_{10}^* \star \eta_{10}\Big]
\end{aligned}$$

which is non-negative by the induction hypothesis. □

Finally we can express the trace of an operator of $\mathcal{B}(\wedge\mathcal{H})$ and due to Lemma 5.20 the trace of a product of such operators as a Grassmann integral.

Theorem 5.29. *For all $A \in \mathcal{B}(\wedge\mathcal{H})$ we have*

$$\mathrm{tr}_{\wedge\mathcal{H}}\,(A) = (-1)^{|M|} \int \mathcal{D}(\overline{\Psi},\Psi)\, \Theta\,(A)\,. \tag{5.22}$$

It is sufficient to assume that A is bounded in Theorem 5.29 for the trace to be finite since $\dim(\mathcal{H}) < \infty$.

Proof. We assume that $A \in \mathcal{B}(\wedge\mathcal{H})$ is normal-ordered. Due to the linearity of the trace and the Grassmann integral it suffices to consider the trace $\mathrm{tr}_{\wedge\mathcal{H}}\left(c_{i_1}^* \cdots c_{i_m}^* c_{j_1} \cdots c_{j_n}\right)$ where $I := \{i_1,\ldots,i_m\}$ and $J := \{j_1,\ldots,j_n\}$ are ordered. For $I \neq J$ both the l.h.s. and the r.h.s. of (5.22) vanish. For $I = J$ the l.h.s. of (5.22) is given by

$$\mathrm{tr}_{\wedge\mathcal{H}}\left(c_{i_1}^* \cdots c_{i_m}^* c_{i_1} \cdots c_{i_m}\right) = (-1)^{\frac{1}{2}|I|(|I|-1)}\, 2^{|M|-|I|}.$$

On the r.h.s. of Equation (5.22) we have $\Theta\left(c_{i_1}^* \cdots c_{i_m}^* c_{i_1} \cdots c_{i_m}\right) = \overline{\psi}_{i_1} \cdots \overline{\psi}_{i_m} \psi_{i_1} \cdots \psi_{i_m}$ and thus

$$\begin{aligned}
\int \mathcal{D}(\overline{\Psi},\Psi)\, \overline{\psi}_{i_1} \cdots \overline{\psi}_{i_m} \psi_{i_1} \cdots \psi_{i_m} &= (-1)^{\frac{1}{2}|I|(|I|+1)} \int \mathcal{D}(\overline{\Psi},\Psi) \prod_{\alpha=1}^{m} \left(\psi_{i_\alpha} \overline{\psi}_{i_\alpha}\right) \\
&= (-1)^{|M|}\, (-1)^{\frac{1}{2}|I|(|I|+1)}\, 2^{|M|-|I|}
\end{aligned}$$

since $\prod_{\alpha\in I}\left(\psi_\alpha \overline{\psi}_\alpha\right) \mathrm{e}^{2(\overline{\Psi},\Psi)} = \prod_{\alpha\in I}\left(\psi_\alpha \overline{\psi}_\alpha\right) \prod_{\alpha\in M\setminus I}\left(1 + 2\overline{\psi}_\alpha \psi_\alpha\right)$ and therefore

$$\prod_{\alpha\in M}\left(\frac{\delta}{\delta\overline{\psi}}\frac{\delta}{\delta\psi}\right) \prod_{\alpha\in I}\left(\psi_\alpha \overline{\psi}_\alpha\right) \mathrm{e}^{2(\overline{\Psi},\Psi)} = (-2)^{|M|-|I|}\,.$$

The proof is complete by $(-2)^{|M|-|I|} = (-1)^{|M|}\, (-1)^{|I|}\, 2^{|M|-|I|}$. □

Due to the restriction to a Hilbert space with even dimension, we henceforth skip the factor $(-1)^{|M|}$.

5 Representability Conditions from Grassmann Integrals

The last section allows for an application of the Grassmann integration on the problem of representability for fermion systems. In particular, we are interested in necessary conditions for the 1- and 2-pdm to have their origin in a density matrix ρ [BKM12]. In the language of Grassmann integration we call the equivalents of density matrices Grassmann densities.

Definition 5.30. A Grassmann variable $\vartheta^* \star \vartheta \in \mathcal{G}_M$ is called Grassmann density if it is normalized, i.e., if it fulfills

$$\int \mathcal{D}\left(\overline{\Psi}, \Psi\right) \vartheta^* \star \vartheta = 1.$$

By definition the Grassmann density is positive semi-definite and self-adjoint. For a given state ρ the map Θ immediately provides $\vartheta^* \star \vartheta$, namely $\vartheta^* \star \vartheta = \Theta(\rho)$. Due to the product rule for Θ and the positive semi-definiteness of ρ we also have $\vartheta^* \star \vartheta = \Theta\left(\rho^{\frac{1}{2}}\rho^{\frac{1}{2}}\right) = \Theta\left(\rho^{\frac{1}{2}}\right) \star \Theta\left(\rho^{\frac{1}{2}}\right)$. Θ is a bijection and compatible with the involution. This implies that $\vartheta = \Theta\left(\rho^{\frac{1}{2}}\right)$. Given a Grassmann density we can formulate the problem of representability by Grassmann integrals using the trace-formula (5.22).

Definition 5.31. Let $\left\{\overline{\psi}_i, \psi_i\right\}_{i\in M}$ be the generators of $\mathcal{G}_M$ and associate $\{\psi_i\}_{i\in M}$ with a fixed ONB of $\mathcal{H}$. The 1-pdm $\gamma_\vartheta \in \mathcal{B}(\mathcal{H})$ and 2-pdm $\Gamma_\vartheta \in \mathcal{B}(\mathcal{H}\otimes\mathcal{H})$ of a Grassmann density $\vartheta^* \star \vartheta$ are defined by their respective matrix elements:

$$\langle \psi_k, \gamma_\vartheta \psi_l \rangle_{\mathcal{H}} := \int \mathcal{D}(\overline{\Psi}, \Psi)\, \vartheta^* \star \vartheta \star \overline{\psi}_l \star \psi_k \quad \text{and} \tag{5.23}$$

$$\langle \psi_m \otimes \psi_n, \Gamma_\vartheta \left(\psi_l \otimes \psi_k\right)\rangle_{\mathcal{H}\otimes\mathcal{H}} := \int \mathcal{D}\left(\overline{\Psi}, \Psi\right) \vartheta^* \star \vartheta \star \overline{\psi}_k \star \overline{\psi}_l \star \psi_m \star \psi_n\,. \tag{5.24}$$

Applying the trace formula (5.22) on (5.23) and (5.24), respectively, we observe that

$$\left\langle \psi_k, \gamma_\rho \psi_l \right\rangle = \mathrm{tr}_{\wedge\mathcal{H}}\left(\Theta^{-1}\left(\vartheta^* \star \vartheta\right) c_l^* c_k\right) \quad \text{and}$$
$$\left\langle \psi_m \otimes \psi_n, \Gamma_\rho\left(\psi_l \otimes \psi_k\right)\right\rangle = \mathrm{tr}_{\wedge\mathcal{H}}\left(\Theta^{-1}\left(\vartheta^* \star \vartheta\right) c_l^* c_k^* c_n c_m\right),$$

which agrees with the common definition of the 1- and 2-pdm [BKM12] if we interpret $\Theta^{-1}\left(\vartheta^* \star \vartheta\right) = \left(\Theta^{-1}(\vartheta)\right)^* \Theta^{-1}(\vartheta)$ as a density matrix $\rho \in \mathcal{B}(\wedge\mathcal{H})$. The problem of representability can be formulated as follows:

Definition 5.32. We call $(\gamma, \Gamma) \in \mathcal{B}(\mathcal{H}) \times \mathcal{B}(\mathcal{H}\otimes\mathcal{H})$ representable if there exists a Grassmann density $\vartheta^* \star \vartheta$ such that $(\gamma, \Gamma) = (\gamma_\vartheta, \Gamma_\vartheta)$.

5.1 Conditions on the One-Particle Density Matrix

The lower and upper bound for the eigenvalues of the 1-pdm γ_ϑ of a Grassmann state $\vartheta^* \star \vartheta$ arise directly from the definition of the 1-pdm (see [BKM12] for further details). Here we would like to derive the conditions by Grassmann integration. To this end we consider certain subspaces of $\mathcal{G}_M$.

Definition 5.33. For any $n \in \mathbb{N}$ with $n \leq |M|$ we define the subspace

$$\mathcal{G}_M^{(n)} := \operatorname{span}\left\{\overline{\Psi}_I \Psi_J \middle| \, |I|, |J| \leq n\right\} \subseteq \mathcal{G}_M.$$

Bounds for the 1-pdm rise by considering $\mathcal{G}_M^{(1)}$ and are called representability conditions of first order. More general, we refer to conditions derived by considering $\mathcal{G}_M^{(n)}$ as representability conditions of n-th order.

Lemma 5.34. *Theorem 5.28 implies*

$$\gamma_\vartheta \geq 0.$$

Proof. Let $\{\overline{\psi}_i, \psi_i\}_{i \in M}$ be the generators of $\mathcal{G}_M$ and $\alpha_k \in \mathbb{C}\ \forall k \in M$. In Theorem 5.28 we make use of Equation (5.18) with $\eta := \phi \star \vartheta^*$ and $\phi := \sum_{k \in M} \alpha_k \psi_k \in \mathcal{G}_M$. We observe that with the involution $(\cdot)^*$ on $\mathcal{G}_M$ $\phi^* = \sum_{k \in M} \overline{\alpha}_k \overline{\psi}_k$ and $\eta^* = (\phi \star \vartheta^*)^* = \vartheta \star \phi^*$. This leads to

$$0 \leq \int \mathcal{D}(\overline{\Psi}, \Psi)\, \eta^* \star \eta = \sum_{k,l \in M} \overline{\alpha}_k \alpha_l \int \mathcal{D}(\overline{\Psi}, \Psi)\, \vartheta^* \star \vartheta \star \overline{\psi}_k \star \psi_l = \langle f, \gamma_\vartheta f \rangle_{\mathcal{H}}$$

where $f := \sum_{i \in M} \overline{\alpha}_i \psi_i \in \mathcal{H}$ is arbitrary. □

The upper bound for γ_ϑ is given by another choice of η.

Lemma 5.35. *Theorem 5.28 implies*

$$\gamma_\vartheta \leq \mathbb{1}.$$

Proof. The bound can be proven by following the steps of the proof of the lower bound. Again, we have $\alpha_k \in \mathbb{C}\ \forall k \in M$ and set $\phi^* = \sum_{k \in M} \overline{\alpha}_k \overline{\psi}_k \in \mathcal{G}_M$ and this time $\eta^* = (\phi^* \star \vartheta)^* = \vartheta^* \star \phi$. Before we go on, we observe that by the CAR on $\mathcal{G}_M$ given in (5.18)

$$\phi \star \phi^* = \sum_{k,l \in M} \alpha_k \overline{\alpha}_l \psi_k \star \overline{\psi}_l = \sum_{k \in M} \overline{\alpha}_k \alpha_k - \sum_{k,l \in M} \alpha_k \overline{\alpha}_l \overline{\psi}_l \star \psi_k.$$

Inserting this into the inequality of Theorem 5.28 and using the associativity of the star product, we obtain

$$\begin{aligned} 0 \leq \int \mathcal{D}(\overline{\Psi}, \Psi)\, \eta^* \star \eta &= \sum_{k \in M} |\alpha_k|^2 - \sum_{k,l \in M} \overline{\alpha}_l \alpha_k \int \mathcal{D}(\overline{\Psi}, \Psi)\, \vartheta^* \star \vartheta \star \overline{\psi}_l \star \psi_k \\ &= \langle g, (\mathbb{1}_{\mathcal{H}} - \gamma_\vartheta)\, g \rangle_{\mathcal{H}} \end{aligned}$$

where we use $\int \mathcal{D}(\overline{\Psi}, \Psi)\, \vartheta^* \star \vartheta = 1$ and $g := \sum_{k \in M} \overline{\alpha}_k \psi_k \in \mathcal{H}$. □

Considering the subspace $\mathcal{G}_M^{(1)}$, we can summarize our last two results.

Theorem 5.36. *Let $\vartheta \star \vartheta^*$ be a Grassmann density and γ_ϑ its 1-pdm. Then the following statements are equivalent:*

a) $0 \leq \gamma_\vartheta \leq \mathbb{1}$.

b) For any $\mu \in \mathcal{G}_M^{(1)}$, $\int \mathcal{D}(\overline{\Psi}, \Psi)\, \vartheta^* \star \vartheta \star \mu \geq 0$ holds.

Proof. In Theorem 3.1 of [BKM12] the analogue of this theorem has been shown for polynomials in creation and annihilation operators of degree lower than or equal to two. Because of the bijection Θ we have a one-to-one mapping between the space of polynomials of degree lower than or equal to two and $\mathcal{G}_M^{(2)}$. □

5.2 G-, P-, and Q-Condition

We proceed with representability conditions of second order by considering $\mathcal{G}_M^{(2)}$ and a star-product of $\overline{\psi}$ and ψ. In this case, for example, $\phi := \sum_{k,l \in M} \alpha_{kl} \psi_k \star \psi_l \in \mathcal{G}_M$ with $\alpha_{kl} \in \mathbb{C}\ \forall k, l \in M$. This time we are interested in conditions on Γ_ϑ and use the Grassmann integration to rewrite the matrix elements of the 2-pdm as in (5.24). The first condition is the P-condition.

Lemma 5.37. *Theorem 5.28 implies the P-condition*

$$\Gamma_\vartheta \geq 0.$$

Proof. The proof is similar to the one in the last subsection. Setting $\phi := \sum_{k,l \in M} \alpha_{kl} \psi_k \star \psi_l \in \mathcal{G}_M$ with $\alpha_{kl} \in \mathbb{C}\ \forall k, l \in M$, $\eta := \phi \star \vartheta^*$, and $\eta^* = (\phi \star \vartheta^*)^* = \vartheta \star \phi^*$, we arrive at

$$\begin{aligned} 0 &\leq \int \mathcal{D}(\overline{\Psi}, \Psi)\, \eta^* \star \eta \\ &= \sum_{k,l,m,n \in M} \overline{\alpha}_{kl} \alpha_{mn} \int \mathcal{D}(\overline{\Psi}, \Psi)\, \vartheta^* \star \vartheta \star \overline{\psi}_l \star \overline{\psi}_k \star \psi_m \star \psi_n \\ &= \langle F, \Gamma_\vartheta F \rangle_{\mathcal{H} \otimes \mathcal{H}} \end{aligned}$$

where $F := \sum_{k,l \in M} \overline{\alpha}_{kl} \left(\psi_m \otimes \psi_n \right) \in \mathcal{H} \otimes \mathcal{H}$ is arbitrary. □

The Q-condition is the next representability condition we consider. In order to obtain a convenient formulation of this condition, we use an exchange operator on $\mathcal{H} \otimes \mathcal{H}$ which is defined by $\mathrm{Ex}\,(f \otimes g) := g \otimes f$ for any $f, g \in \mathcal{H}$.

Lemma 5.38. *Theorem 5.28 implies the Q-condition*

$$\Gamma_\vartheta + \left(\mathbb{1}_{\mathcal{H} \otimes \mathcal{H}} - \mathrm{Ex} \right) \left(\mathbb{1}_\mathcal{H} \otimes \mathbb{1}_\mathcal{H} - \gamma_\vartheta \otimes \mathbb{1}_\mathcal{H} - \mathbb{1}_\mathcal{H} \otimes \gamma_\vartheta \right) \geq 0.$$

Proof. With $\phi := \sum_{k,l\in M} \overline{\alpha}_{kl} \overline{\psi}_k \star \overline{\psi}_l \in \mathcal{G}_M$, $\alpha_{kl} \in \mathbb{C}\ \forall k,l \in M$, and $\eta = \phi \star \vartheta^*$ we have

$$
\begin{aligned}
0 &\le \int \mathcal{D}(\overline{\Psi},\Psi)\, \eta^* \star \eta \\
&= \sum_{k,l,m,n\in M} \overline{\alpha}_{kl}\alpha_{mn} \int \mathcal{D}(\overline{\Psi},\Psi)\, \vartheta^* \star \vartheta \star \psi_n \star \psi_m \star \overline{\psi}_k \star \overline{\psi}_l .
\end{aligned}
$$

Aiming for an expression in terms of Γ and γ, we establish normal ordering using the CAR:

$$
\begin{aligned}
\psi_n \star \psi_m \star \overline{\psi}_k \star \overline{\psi}_l =& \delta_{mk}\delta_{nl} - \delta_{nk}\delta_{ml} + \delta_{nk}\overline{\psi}_l \star \psi_m - \delta_{mk}\overline{\psi}_l \star \psi_n + \delta_{nl}\overline{\psi}_k \star \psi_l \\
&- \delta_{ml}\overline{\psi}_k \star \psi_n - \overline{\psi}_k \star \overline{\psi}_l \star \psi_n \star \psi_m . \qquad (5.25)
\end{aligned}
$$

As in the proof of Lemma 5.37 we write an arbitrary $G \in \mathcal{H}\otimes\mathcal{H}$ as $G := \sum_{k,l\in M} \alpha_{kl} \left(\psi_k \otimes \psi_l\right)$ for some $\alpha_{kl} \in \mathbb{C}$. Hence, $\sum_{k,l,m,n\in M} \overline{\alpha}_{kl}\alpha_{mn}\delta_{km}\delta_{ln} = \langle G, \mathbb{1}_{\mathcal{H}\otimes\mathcal{H}} G\rangle_{\mathcal{H}\otimes\mathcal{H}}$ and $\sum_{k,l,m,n\in M} \overline{\alpha}_{kl}\alpha_{mn}\delta_{kn}\delta_{lm} = \langle G, \mathrm{Ex}\, G\rangle_{\mathcal{H}\otimes\mathcal{H}}$. With (5.23) and (5.24) we find

$$
0 \le \langle G, \left(\Gamma_\vartheta + \left(\mathbb{1}_{\mathcal{H}\otimes\mathcal{H}} - \mathrm{Ex}\right)\left(\mathbb{1}_{\mathcal{H}} \otimes \mathbb{1}_{\mathcal{H}} - \gamma_\vartheta \otimes \mathbb{1}_{\mathcal{H}} - \mathbb{1}_{\mathcal{H}} \otimes \gamma_\vartheta\right)\right) G\rangle_{\mathcal{H}\otimes\mathcal{H}}
$$

by evaluating the Grassmann integral $\int \mathcal{D}(\overline{\Psi},\Psi)\,(\cdot)$ on the r.h.s. of Equation (5.25). □

The last second order representability condition which can be derived by the described method is the (optimal) G-condition. Deriving this condition by Grassmann integration requires a choice of η that is not as obvious as before.

Lemma 5.39. *Theorem 5.28 implies the G-condition:*

$$
\mathrm{tr}_{\mathcal{H}\otimes\mathcal{H}}\left(\left(A^* \otimes A\right)\left(\Gamma_\vartheta + \mathrm{Ex}\left(\gamma_\vartheta \otimes \mathbb{1}_{\mathcal{H}}\right)\right)\right) \ge \left|\mathrm{tr}_{\mathcal{H}}\left(A\gamma_\vartheta\right)\right|^2
$$

for any $A \in \mathcal{B}(\mathcal{H}\otimes\mathcal{H})$.

Proof. This time we choose $\eta := \left(\sum_{k,l\in M} \alpha_{kl}\overline{\psi}_k \star \psi_l - c\right) \star \vartheta$ with $\alpha_{kl} \in \mathbb{C}$ for all $k,l \in M$ and $c := \sum_{k,l\in M} \alpha_{kl} \int \mathcal{D}(\overline{\Psi},\Psi)\, \vartheta^* \star \vartheta \star \overline{\psi}_k \star \psi_l$. Before we apply Theorem 5.28, we emphasize that by the CAR

$$
\begin{aligned}
&\left(\sum_{k,l\in M} \alpha_{kl}\overline{\psi}_k\psi_l - c\right)^* \star \left(\sum_{k,l\in M} \alpha_{kl}\overline{\psi}_k\psi_l - c\right) \\
&\qquad = \overline{c}c - c\sum_{k,l\in M} \overline{\alpha}_{kl}\overline{\psi}_l \star \psi_k - \overline{c}\sum_{m,n\in M} \alpha_{mn}\overline{\psi}_m \star \psi_n \\
&\qquad\quad - \sum_{k,l\in M} \overline{\alpha}_{kl}\alpha_{mn}\overline{\psi}_l \star \overline{\psi}_m \star \psi_k \star \psi_n + \sum_{k,l,n\in M} \overline{\alpha}_{kl}\alpha_{kn}\overline{\psi}_l \star \psi_n .
\end{aligned} \qquad (5.26)
$$

We consider the last two lines separately and integrate. The integration of the line before the last line in (5.26) yields

$$
\begin{aligned}
&\int \mathcal{D}(\overline{\Psi},\Psi)\, \vartheta^* \star \vartheta \star \left(\overline{c}c - c\sum_{k,l\in M} \overline{\alpha}_{kl}\overline{\psi}_l \star \psi_k - \overline{c}\sum_{m,n\in M} \alpha_{mn}\overline{\psi}_m \star \psi_n\right) \\
&\qquad = \overline{c}c - c\overline{c} - \overline{c}c = -\overline{c}c
\end{aligned} \qquad (5.27)
$$

which follows from the definition of c. It is important to notice that c does not depend on ψ or $\overline{\psi}$ and therefore is a constant with respect to the Grassmann integration. In detail we have for c:

$$c = \sum_{k,l \in M} \alpha_{kl} \int \mathcal{D}(\overline{\Psi}, \Psi)\, \vartheta^* \star \vartheta \star \overline{\psi}_k \star \psi_l = \mathrm{tr}_{\mathcal{H}} \left(A \gamma_\vartheta \right) \tag{5.28}$$

if we define $A \in \mathcal{B}(\mathcal{H})$ by $\langle \psi_k, A\psi_l \rangle_{\mathcal{H}} := \alpha_{kl}$ for every $k, l \in M$. The evaluation of the Grassmann integral of the last line in (5.26) provides

$$\begin{aligned} - \sum_{k,l \in M} \overline{\alpha}_{kl} \alpha_{mn} \int \mathcal{D}(\overline{\Psi}, \Psi)\, \vartheta^* \star \vartheta \star \overline{\psi}_l \star \overline{\psi}_m \star \psi_k \star \psi_n & \\ + \sum_{k,l,n \in M} \overline{\alpha}_{kl} \alpha_{kn} \int \mathcal{D}(\overline{\Psi}, \Psi)\, \vartheta^* \star \vartheta \star \overline{\psi}_l \star \psi_n & \\ = \mathrm{tr}_{\mathcal{H} \otimes \mathcal{H}} \left((A^* \otimes A) \left(\Gamma_\vartheta + \mathrm{Ex} \left(\gamma_\vartheta \otimes \mathbb{1}_{\mathcal{H}} \right) \right) \right). & \end{aligned} \tag{5.29}$$

Summing up, calculation (5.27) together with (5.28) and (5.29) gives

$$\mathrm{tr}_{\mathcal{H} \otimes \mathcal{H}} \left((A^* \otimes A) \left(\Gamma_\vartheta + \mathrm{Ex} \left(\gamma_\vartheta \otimes \mathbb{1}_{\mathcal{H}} \right) \right) \right) - \left| \mathrm{tr}_{\mathcal{H}} \left(A \gamma_\vartheta \right) \right|^2 \geq 0$$

by Theorem 5.28. □

We summarize our results using $\mathcal{G}_M^{(2)}$:

Theorem 5.40. *Let $\vartheta \star \vartheta^*$ be a Grassmann density, γ_ϑ its 1-pdm, and Γ_ϑ its 2-pdm. Then the following statements are equivalent:*

a) $(\gamma_\vartheta, \Gamma_\vartheta)$ fulfills $0 \leq \gamma_\vartheta \leq \mathbb{1}$ and the G-, P-, and Q-conditions.

b) For any $\mu \in \mathcal{G}_M^{(2)}$ $\int \mathcal{D}(\overline{\Psi}, \Psi)\, \vartheta^* \star \vartheta \star \mu \geq 0$ holds.

Proof. Again we use Theorem 3.1 of [BKM12] and the bijection property of Θ which ensures that the space of polynomials of degree lower or equal than four in creation and annihilation operators is mapped one-to-one to $\mathcal{G}_M^{(2)}$. □

5.3 T_1- and Generalized T_2-Condition

The last sections imply that further conditions on γ_ϑ and Γ_ϑ can be found by taking into account monomials of higher order of the form $\overline{\psi}_{i_1} \star \cdots \star \overline{\psi}_{i_n} \star \psi_{j_1} \star \cdots \star \psi_{j_n}$ for $n > 2$. Here we face the problem that monomials with $n > 2$ have to "decompose" into monomials with $n \leq 2$. Due to this only some choices of higher order monomials are suitable to derive further representability conditions. One such monomial is given by

$$\tau_1 := \sum_{i,j,k \in M} T_{ijk} \psi_i \star \psi_j \star \psi_k \in \mathcal{G}_M$$

where $T_{ijk} \in \mathbb{C}$ is totally antisymmetric due to $\left\{ \psi_i, \psi_j \right\}_\star = 0$, i.e., $T_{ijk} = -T_{jik} = T_{jki}$. The T_1-condition is the following.

Theorem 5.41. *Let $T_q \in \mathcal{B}(\mathcal{H})$ be trace-class and set $T_{kqn} := [T_q]_{kn}$, $F_{T_q} := \sum_{k,n\in M} \overline{T}_{kqn} (\varphi_k \otimes \varphi_n) \in \mathcal{H} \otimes \mathcal{H}$. Then Theorem 5.28 implies the* T_1*-condition:*

$$\sum_{q\in M} \left(2\mathrm{tr}_{\mathfrak{h}} \left(|T_q|^2 \right) - 6\mathrm{tr}_{\mathfrak{h}} \left(|T_q|^2 \gamma_\vartheta \right) + 3 \left\langle F_{T_q}, \Gamma_\vartheta F_{T_q} \right\rangle \right) \geq 0.$$

Proof. We begin by considering the anticommutator $\{\tau_1^*, \tau_1\}_\star \in \mathcal{G}_M$ and observe that by construction $\{\tau_1^*, \tau_1\}_\star \geq 0$. Furthermore we can use the CAR to establish normal order in $\{\tau_1^*, \tau_1\}_\star$. The $i,j-$th matrix element of $A \in \mathcal{B}(\mathcal{H})$ is denoted by $[A]_{ij} := \langle \psi_i, A\psi_j \rangle_{\mathcal{H}}$. Using the antisymmetry of T_{ijk} we arrive at

$$\begin{aligned}
\{\tau_1^*, \tau_1\}_\star &= 9 \sum_{l\in M} \sum_{i,j,m,n\in M} \overline{T}_{ljm} T_{lin} \overline{\psi}_m \star \overline{\psi}_j \star \psi_i \star \psi_n \\
&\quad + 18 \sum_{m,l\in M} \sum_{k,n\in M} \overline{T}_{kml} T_{lmn} \overline{\psi}_k \star \psi_n + 6 \sum_{l,m,n\in M} \overline{T}_{lmn} M_{lmn} \\
&= 9 \sum_{q\in M} \sum_{i,j,m,n\in M} \left[T_q^* \right]_{mj} [T_q]_{in} \overline{\psi}_m \star \overline{\psi}_j \star \psi_i \star \psi_n \\
&\quad - 18 \sum_{q\in M} \sum_{k,n\in M} \left[T_q^* T_q \right]_{kn} \overline{\psi}_k \star \psi_n + 6 \sum_{q\in M} \mathrm{tr}_{\mathfrak{h}} \left(|T_q|^2 \right).
\end{aligned}$$

Since $\{\tau_1^*, \tau_1\}_\star \geq 0$, we have by Theorem 5.28

$$\int \mathcal{D}(\overline{\Psi}, \Psi)\, \vartheta \star \{\tau_1^*, \tau_1\}_\star \star \vartheta^* \geq 0.$$

Together with (5.24) the latter calculations and this non-negativity of the integral bring us to

$$\begin{aligned}
0 \leq\, & 3 \sum_{q\in M} \sum_{i,j,m,n\in M} \left[T_q^* \right]_{mj} [T_q]_{in} \langle \psi_i \otimes \psi_n, \Gamma_\vartheta (\psi_j \otimes \psi_m) \rangle \\
& - 6 \sum_{q\in M} \sum_{k,n\in M} \left[|T_q|^2 \right]_{kn} \langle \psi_n, \gamma_\vartheta \psi_k \rangle + 2 \sum_{q\in M} \mathrm{tr}_{\mathfrak{h}} \left(|T_q|^2 \right).
\end{aligned}$$

Together with $\langle \psi_i, T_q \psi_j \rangle =: [T_q]_{ij}$ and $F_{T_q} := \sum_{k,n\in M} \overline{T}_{kqn} (\varphi_k \otimes \varphi_n)$ this yields the assertion. □

The generalized T_2-condition can be derived equivalently by another choice of τ. Using the anticommutator with a combination of two $\overline{\psi}$'s and one ψ (or vice versa), we have three different possibilities:

$$\begin{aligned}
\tau_{2a} &:= \sum_{i,j,k\in M} T_{ijk}^{(a)} \overline{\psi}_i \star \overline{\psi}_j \star \psi_k, \\
\tau_{2b} &:= \sum_{i,j,k\in M} T_{ijk}^{(b)} \overline{\psi}_i \star \psi_j \star \overline{\psi}_k, \text{ and} \\
\tau_{2c} &:= \sum_{i,j,k\in M} T_{ijk}^{(c)} \psi_i \star \overline{\psi}_j \star \overline{\psi}_k.
\end{aligned}$$

A generalization of these possibilities is given by

$$\tau_2 := \sum_{i,j,k\in M} T_{ijk}\overline{\psi}_i \star \overline{\psi}_j \star \psi_k + \sum_{i\in M} a_i \overline{\psi}_i$$

where T_{ijk}, $a_i \in \mathbb{C}$ for all $i, j, k \in M$. This is a generalization since we obtain $\tau_2 = \tau_{2a}$ for $\alpha_i \equiv 0$ and $T_{ijk} \equiv T^{(a)}_{ijk}$, $\tau_2 = \tau_{2b}$ for $a_i = \sum_{j\in M} T^{(b)}_{ijj}$ and $T_{ijk} = -T^{(b)}_{ikj}$, and finally $\tau_2 = \tau_{2c}$ for $a_i = \sum_{j\in M}\left(T^{(c)}_{jji} - T^{(c)}_{jij}\right)$ and $T_{ijk} = T^{(c)}_{kij}$. The identities can be seen by using the CAR. Unfortunately, if one uses the generalization τ_2, symmetry properties on T_{ijk} like, for example, $T^{(a)}_{ijk} = -T^{(a)}_{jik}$ in τ_{2a} or $T^{(c)}_{ijk} = -T^{(c)}_{ikj}$ in τ_{2c} vanish. The generalized T_2-condition rises from $\{\tau_2^*, \tau_2\}_\star \geq 0$. In order to state the condition in a compact form, we need some new notation.

Definition 5.42. For $T_k \in \mathcal{B}(\mathcal{H})$, $[T_k]_{ij} := T_{ijk}$ for each $i, j, k \in M$, and $\underline{a} \in \mathbb{C}^{|M|}$ we define $G_{M_k} \in \mathcal{H}\otimes\mathcal{H}$ and the matrices $Q_1 \in \mathcal{B}(\mathcal{H}\otimes\mathcal{H})$ and Q_2, $Q_3 \in \mathcal{B}(\mathcal{H})$ by

$$G_{M_k} := \sum_{i,j\in M} [T_k]_{ij}\left(\psi_i \otimes \psi_j\right),$$

$$\left\langle \psi_k \otimes \psi_m, Q_1\left(\psi_n\otimes\psi_j\right)\right\rangle_{\mathcal{H}\otimes\mathcal{H}} := \left[\overline{T}^{(A)}_k T^{(A)}_n\right]_{jm},$$

$$\left\langle \psi_i, Q_2 \psi_j\right\rangle_{\mathcal{H}} := \mathrm{tr}_{\mathcal{H}}\left(\left(T^{(A)}_i\right)^* T_j\right),$$

$$\left\langle \psi_i, Q_3 \psi_j\right\rangle_{\mathcal{H}} := \sum_{q\in M}\left(\left[\left(T^{(A)}_i\right)^*\right]_{jq} a_q + \left[T^{(A)}_j\right]_{iq}\overline{a}_q\right)$$

where $\left[T^{(A)}_k\right]_{ij} := \frac{1}{2}\left([T_k]_{ij} - [T_k]_{ji}\right) = -\left[T^{(A)}_k\right]_{ji}$ is the antisymmetric part of T_k.

Theorem 5.43. *Let T_k, $\underline{a}$, G_{T_q} and Q_1, Q_2, Q_3 be as in Definition 5.42. Then Theorem 5.28 implies the generalized T_2-condition:*

$$\sum_{q\in M}\left\langle G_{T_q}, \Gamma_\vartheta G_{T_q}\right\rangle_{\mathcal{H}\otimes\mathcal{H}} + 4\mathrm{tr}_{\mathcal{H}\otimes\mathcal{H}}\left(Q_1\Gamma_\vartheta\right) + 2\mathrm{tr}_{\mathcal{H}}\left(\left(Q_2+Q_3\right)\gamma_\vartheta\right) + |\underline{a}|^2 \geq 0.$$

Proof. The first task is to bring $\{\tau_2^*, \tau_2\}$ into normal order. Afterwards the two terms of third order cancel. Only terms of order less than or equal to two remain. We use $\left\{(\mu+\eta)^*, \mu+\eta\right\}_\star = \{\mu^*, \mu\}_\star + 2\mathfrak{Re}\,\{\mu^*, \eta\}_\star + \{\eta^*, \eta\}_\star$ for $\mu := \sum_{i,j,k\in M} T_{ijk}\overline{\psi}_i \star \overline{\psi}_j \star \psi_k$ and $\eta := \sum_{i\in M} a_i\overline{\psi}_i$ to calculate the anticommutator. By the CAR we have

$$\{\eta^*, \eta\}_\star = \sum_{i\in M} |a_i|^2, \qquad \{\mu^*, \eta\}_\star = \sum_{k,n\in M}\sum_{q\in M}\left(\overline{T}_{qnk} - \overline{T}_{nqk}\right) a_q \overline{\psi}_k \star \psi_n$$

and

$$\{\mu^*, \mu\}_\star = \sum_{j,k,m,n \in M} \sum_{q \in M} \Big(\left(\overline{T}_{jqk} - \overline{T}_{qjk} \right) \left(T_{qmn} - T_{mqn} \right) + \overline{T}_{njq} T_{kmq} \Big) \overline{\psi}_k \star \overline{\psi}_m \star \psi_j \star \psi_n + \sum_{k,n \in M} \sum_{p,q \in M} \left(\overline{T}_{pqk} - \overline{T}_{qpk} \right) T_{pqn} \overline{\psi}_k \star \psi_n .$$

We set $T_{ijq} =: [T_q]_{ij}$ where $T_q \in \mathcal{B}(\mathcal{H})$ for any $q \in M$ and observe that $\left[\overline{T}_q\right]_{ij} = \left[T_q^*\right]_{ji}$, $\overline{T}_{qnk} - \overline{T}_{nqk} = 2\left[\left(T_k^{(A)}\right)^*\right]_{nq}$, and $T_{qmn} - T_{mqn} = 2\left[T_n^{(A)}\right]_{qm}$ where $T^{(A)}$ is the antisymmetric part of T (see Definition 5.42). This allows us to rewrite the anticommutators:

$$2\mathfrak{Re}\,\{\mu^*, \eta\}_\star = 2 \sum_{k,n \in M} \sum_{q \in M} \left(\left[\left(T_k^{(A)}\right)^*\right]_{nq} a_q + \left[T_n^{(A)}\right]_{qk} \overline{a}_q \right) \overline{\psi}_k \star \psi_n$$

and

$$\{\mu^*, \mu\}_\star = \sum_{j,k,m,n \in M} \sum_{q \in M} \left(4 \left[\left(T_k^{(A)}\right)^*\right]_{qj} \left[T_n^{(A)}\right]_{qm} + \left[T_q^*\right]_{jn} \left[T_q\right]_{km} \right) \overline{\psi}_k \star \overline{\psi}_m \star \psi_j \star \psi_n + 2 \sum_{k,n \in M} \sum_{p,q \in M} \left[\left(T_k^{(A)}\right)^*\right]_{qp} \left[T_n\right]_{pq} \overline{\psi}_k \star \psi_n . \tag{5.30}$$

In the next step we use the notation $\langle \psi_i, A\psi_j \rangle_{\mathcal{H}} = [A]_{ij}$ for $A \in \mathcal{B}(\mathcal{H})$ and the Grassmann representation of γ and Γ from (5.23) and (5.24). Definition 5.42 then leads to

$$\sum_{j,k,m,n \in M} \sum_{q \in M} \left[T_q^*\right]_{jn} \left[T_q\right]_{km} \int \mathcal{D}(\overline{\Psi}, \Psi)\, \vartheta^* \star \vartheta \star \overline{\psi}_k \star \overline{\psi}_m \star \psi_j \star \psi_n = \sum_{q \in M} \left\langle G_{T_q}, \Gamma_\vartheta G_{T_q} \right\rangle_{\mathcal{H}\otimes\mathcal{H}}$$

for $G_{T_q} := \sum_{i,j \in M} \left[T_q\right]_{ij} \left(\psi_i \otimes \psi_j\right) \in \mathcal{H} \otimes \mathcal{H}$. Moreover we have by the definition of Q_1 as $\langle \psi_m \otimes \psi_k, Q_1 \left(\psi_j \otimes \psi_n\right) \rangle_{\mathcal{H}\otimes\mathcal{H}} := \left[\overline{T}_k^{(A)} T_n^{(A)}\right]_{jm}$

$$4 \sum_{j,k,m,n,q \in M} \left[\overline{T}_k^{(A)}\right]_{jq} \left[T_n^{(A)}\right]_{qm} \int \mathcal{D}(\overline{\Psi}, \Psi)\, \vartheta^* \star \vartheta \star \overline{\psi}_k \star \overline{\psi}_m \star \psi_j \star \psi_n = 4\mathrm{tr}_{\mathcal{H}\otimes\mathcal{H}} \left(Q_1 \Gamma_\vartheta\right).$$

Furthermore

$$2 \sum_{k,n \in M} \sum_{p,q \in M} \left[\left(T_k^{(A)}\right)^*\right]_{qp} \left[T_n\right]_{pq} \int \mathcal{D}(\overline{\Psi}, \Psi)\, \vartheta^* \star \vartheta \star \overline{\psi}_k \star \psi_n = 2\mathrm{tr}_{\mathcal{H}} \left(Q_2 \gamma_\vartheta\right)$$

for $[Q_2]_{kn} := \mathrm{tr}_{\mathcal{H}}\left(\left(T_k^{(A)}\right)^* T_n\right)$.

With $[Q_3]_{ij} := \sum_{q\in M}\left(\left[\left(T_i^{(A)}\right)^*\right]_{jq} a_q + \left[T_j^{(A)}\right]_{qi} \overline{a}_q\right)$ we finally obtain

$$2\mathfrak{Re}\int \mathcal{D}(\overline{\Psi},\Psi)\,\vartheta^* \star \vartheta \star \{\mu^*,\eta\}_\star = 2\mathrm{tr}_{\mathcal{H}}\left(Q_3\gamma_\vartheta\right).$$

$\sum_i |a_i|^2 =: |\underline{a}|^2$ is the squared Euclidean norm of $\underline{a}$. The proof is complete by inserting the latter calculations into the inequality of Theorem 5.28. □

As already mentioned, we have antisymmetry properties for certain choices of $\underline{a}$ and T_{ijk}. In τ_{2a}, which we obtain by setting $\underline{a} \equiv 0$ and $T_{ijk} = T_{ijk}^{(a)} = \left[T_k^{(a)}\right]_{ij}$, we have $[T_k]_{ij} = -[T_k]_{ji}$ or $T_k \equiv T_k^{(A)}$. In this case we have a simplification of the generalized T_2-condition:

Corollary 5.44. *For $\underline{a} \equiv 0$, $T_k \equiv T_k^{(A)}$, and $\left[\tilde{T}_k\right]_{ij} := \left[T_j\right]_{ik}$, we have the T_{2a}-condition given by*

$$\sum_{q\in M}\left(\langle G_{\tilde{T}_q}, \Gamma_\vartheta G_{\tilde{T}_q}\rangle_{\mathcal{H}\otimes\mathcal{H}} + 4\mathrm{tr}_{\mathcal{H}\otimes\mathcal{H}}\left(\left(\tilde{T}_q^* \otimes \tilde{T}_q\right)\Gamma_\vartheta\right) + 2\mathrm{tr}_{\mathcal{H}}\left(\left|\tilde{T}_q\right|^2 \gamma_\vartheta\right)\right) \geq 0.$$

Proof. With $\underline{a} \equiv 0$ we only have to consider $\{\mu^*,\mu\}_\star$ and can use (5.30) with $T_k \equiv T_k^{(A)}$. □

We can also use an antisymmetry property in τ_{2c} which leads to a condition T_{2c}. Unfortunately there is no simplification compared to the generalized T_2-condition. There is, however, no antisymmetry property in τ_{2b}. Since $\{\tau_1^*,\tau_1\}_\star, \{\tau_2^*,\tau_2\}_\star \in \mathcal{G}_M^{(3)}$, the T_1- and T_2-conditions are representability conditions of third order.

6 Quasifree Grassmann States

The notion of Grassmann integration allows for a calculation of traces on the fermion Fock space by Grassmann integrals and in turn to reformulate representability condition in terms of Grassmann integrals. At last we consider quasifree states, their one-particle density matrices, and the expression of their relation in terms of Grassmann integrals.

In the following we will abbreviate the expectation value of a Grassmann variable $\mu \in \mathcal{G}_M$ with respect to a Grassmann density $\varkappa \in \mathcal{G}_M$ by

$$\int \mathcal{D}(\overline{\Psi},\Psi)\,\varkappa \star \mu =: \langle\,\mu\,\rangle_\varkappa.$$

Definition 5.45. Let $N \in \mathbb{N}$ and $\widetilde{\psi}_i$ denote either $\psi_i \in \mathcal{G}_M$ or $\overline{\psi}_i \in \mathcal{G}_M$ where $\{\overline{\psi}_i, \psi_i\}_{i\in M}$ is a set of generators of $\mathcal{G}_M$. We call a Grassmann density $\varkappa$ quasifree if

1) $\left\langle \widetilde{\psi}_1 \star \widetilde{\psi}_2 \star \cdots \star \widetilde{\psi}_{2N-1}\right\rangle_\varkappa = 0$ and

2) $\langle \widetilde{\psi}_1 \star \widetilde{\psi}_2 \star \cdots \star \widetilde{\psi}_{2N} \rangle_\varkappa$
$$= \sum_{\pi}{}' (-1)^\pi \left\langle \widetilde{\psi}_{\pi(1)} \star \widetilde{\psi}_{\pi(2)} \right\rangle_\varkappa \times \cdots \times \left\langle \widetilde{\psi}_{\pi(2N-1)} \star \widetilde{\psi}_{\pi(2N)} \right\rangle_\varkappa$$

where $\sum_\pi{}'$ denotes the sum over all permutations π obeying $\pi(1) < \pi(3) < \cdots < \pi(2N-1)$ and $\pi(2j-1) < \pi(2j)$ for all $1 \le j \le N$. The maximal number of (distinct) ψ_i or $\overline{\psi}_i$ in 1) and 2) is less or equal $|M|$.

Remark 5.46. We have to restrict N in the latter definition or extend M sufficiently since the expressions on the l.h.s. of conditions 1) and 2) vanish if the number of ψ_i or $\overline{\psi}_i$ is larger than $|M|$.

As it is already known from [BLS94], there is a unique characterization of quasifree states by the 1-pdm. More precisely, assuming particle number-conservation and defining

$$\widetilde{\gamma} := \begin{pmatrix} \gamma & 0 \\ 0 & \mathbb{1}_\mathcal{H} - \overline{\gamma} \end{pmatrix} \in \mathcal{B}(\mathcal{H} \oplus \mathcal{H}),$$

which is the generalized 1-pdm corresponding to γ, one has the following theorem.

Theorem 5.47. *Let* $\widetilde{\gamma} = \left(\begin{smallmatrix} \gamma & 0 \\ 0 & \mathbb{1}_\mathcal{H} - \overline{\gamma} \end{smallmatrix}\right)$ *be an operator on* $\mathcal{H} \oplus \mathcal{H}$ *with* $\mathrm{tr}_\mathcal{H}(\gamma) < \infty$ *and* $0 \le \widetilde{\gamma} \le \mathbb{1}_{\mathcal{H}\oplus\mathcal{H}}$. *Then there exists a unique quasifree state* ρ *with* $\mathrm{tr}_{\wedge\mathcal{H}}\left(\rho\widehat{\mathbb{N}}\right) < \infty$ *such that* $\widetilde{\gamma} = \widetilde{\gamma}_\rho$.

For a proof see [BLS94].

In the language of Grassmann integration the reverse direction, namely that $\widetilde{\gamma}_\varkappa$, i.e., the generalized 1-pdm of a quasifree Grassmann density $\varkappa$, has to fulfill $0 \le \widetilde{\gamma}_\varkappa \le \mathbb{1}_{\mathcal{H}\oplus\mathcal{H}}$, can be deduced by appropriate choices of $\phi \in \mathcal{G}_M$ in the positivity condition

$$\langle \phi^* \star \phi \rangle_\varkappa \ge 0.$$

The aim of this section is to determine the unique quasifree Grassmann density subject to Theorem 5.47, i.e., the element of a Grassmann algebra corresponding the state given in [BLS94]. To this end we consider an operator $\widetilde{\gamma} \in \mathcal{B}(\mathcal{H} \oplus \mathcal{H})$ with $0 \le \widetilde{\gamma} \le \mathbb{1}_{\mathcal{H}\oplus\mathcal{H}}$ and its eigenvalues λ_i and $(1-\lambda_i)$ where $0 \le \lambda_i \le \frac{1}{2}$ for any $i \in M$. Furthermore we define P_0 to be the projection onto the subspace of $\wedge\mathcal{H}$ on which $\sum_{i\in M:\lambda_i=0} c_i^* c_i = 0$. Moreover for any $i \in M$ the quantity q_i is given by the relation $(1+\mathrm{e}^{q_i})^{-1} = \lambda_i$. Then according to [BLS94] any operator $\widetilde{\gamma}$ with $0 \le \widetilde{\gamma} \le \mathbb{1}_{\mathcal{H}\oplus\mathcal{H}}$ is the generalized 1-pdm of a unique quasifree state $\rho \in \mathcal{B}(\wedge\mathcal{H})$ given by

$$\rho := \frac{G}{\mathrm{tr}_{\wedge\mathcal{H}}(G)} \tag{5.31}$$

where

$$G := P_0 \mathrm{e}^{-H} \quad \text{and} \quad H := \sum_{i\in M:\lambda_i\neq 0} q_i c_i^* c_i.$$

Before we turn to the definition of the Grassmann density corresponding to (5.31), we introduce the abbreviations $\Theta_0 := \Theta(P_0) \in \mathcal{G}_M$ and $\prod_{i=1}^{n}{}^{\star}\mu_i := \mu_1 \star \mu_2 \star \cdots \star \mu_n$ for $\mu_i \in \mathcal{G}_M$. Furthermore we associate the generators $\{\overline{\psi}_i, \psi_i\}_{i\in M}$ of $\mathcal{G}_M$ with the ONB $\{\psi_i\}_{i\in M}$ of $\mathcal{H}$ where the ψ_i are the eigenvectors of γ corresponding to the eigenvalues λ_i and $(1-\lambda_i)$.

Lemma 5.48. *Let $\{\psi_i\}_{i\in M}$ be an ONB of $\mathcal{H}$ such that $\gamma\psi_i = \lambda_i\psi_i$ and let $\mathcal{G}_M$ be generated by $\{\overline{\psi}_i, \psi_i\}_{i\in M}$. The Grassmann density $\varkappa \in \mathcal{G}_M$ corresponding to $\rho = \frac{G}{\mathrm{tr}_{\wedge\mathcal{H}}(G)}$ is given by*

$$\varkappa = \frac{1}{Z}\left(\Theta_0 \star \prod_{i\in M:\lambda_i\neq 0}{}^{\star}\left(\left(\mathrm{e}^{-q_i}-1\right)\overline{\psi}_i\psi_i + 1\right)\right), \tag{5.32}$$

where

$$Z := \int \mathcal{D}(\overline{\Psi},\Psi)\,\Theta_0 \star \prod_{i:\lambda_i\neq 0}{}^{\star}\left(\left(\mathrm{e}^{-q_i}-1\right)\overline{\psi}_i\psi_i + 1\right).$$

Proof. We consider $\Theta(\rho)$ subject to (5.31). We first observe that $c_i^* c_i$ commutes with $c_k^* c_k$ for every i, k. Therefore we have

$$\mathrm{e}^{-H} = \prod_{i\in M:\lambda_i\neq 0}\left(\sum_{n=1}^{\infty}\frac{(-q_i)^n}{n!}c_i^* c_i + 1\right) = \prod_{i\in M:\lambda_i\neq 0}\left(\left(\mathrm{e}^{-q_i}-1\right)c_i^* c_i + 1\right)$$

since $\left(c_i^* c_i\right)^n = c_i^* c_i$. Thus,

$$\begin{aligned}\Theta\left(P_0\mathrm{e}^{-H}\right) &= \Theta_0 \star \Theta\left(\prod_{i\in M:\lambda_i\neq 0}\left(\left(\mathrm{e}^{-q_i}-1\right)c_i^* c_i + 1\right)\right)\\ &= \Theta_0 \star \prod_{i\in M:\lambda_i\neq 0}{}^{\star}\left(\left(\mathrm{e}^{-q_i}-1\right)\overline{\psi}_i\psi_i + 1\right)\end{aligned}$$

where we have used that $\Theta(AB) = \Theta(A) \star \Theta(B)$. □

The Grassmann state corresponding to the Grassmann density (5.32) is given by the map

$$\mathcal{G}_M \to \mathbb{C}, \quad \mu \mapsto \langle \mu \rangle_{\varkappa}.$$

We want to verify that the Grassmann density from Lemma 5.48 is quasifree, i.e., that it fulfills conditions 1) and 2) from Definition 5.45. The uniqueness of $\varkappa$ follows from the bijection property of the map Θ.

Theorem 5.49. *The Grassmann state $\varkappa$ given in Lemma 5.48 is quasifree.*

Proof. We consider the state

$$\varkappa_\mu := \prod_{i\in M}{}^{\star}\left(r_i\overline{\psi}_i\psi_i + 1\right)$$

where $r_i := \mathrm{e}^{-q_i(\mu)} - 1$ and $q_i(\mu) \equiv \mu \in \mathbb{R}$ for all i with $\lambda_i = 0$ and $q_i(\mu) \equiv q_i$ for all i with $\lambda_i \neq 0$. The quasifreeness of $\varkappa$ follows by the quasifreeness of $\varkappa_\mu$ and a limiting argument. The first claim of Definition 5.45 is immediate for $\varkappa_\mu$ since the Grassmann integral vanishes for an odd number of $\widetilde{\psi}$'s. This can be seen by Remark 5.25 and the chequerboard. The validity of Equation 2) of Definition 5.45 has already been proven in [Gau60]. Here we emphasize the main steps and transfer the notation of [Gau60] to Grassmann Integrals. We consider the l.h.s. of claim 2) of Definition 5.45,

$$\left\langle \widetilde{\psi}_a \star \widetilde{\psi}_b \star \widetilde{\psi}_c \star \cdots \star \widetilde{\psi}_f \right\rangle_{\varkappa_\mu} = \int \mathcal{D}(\overline{\Psi}, \Psi)\, \varkappa_\mu \star \widetilde{\psi}_a \star \widetilde{\psi}_b \star \widetilde{\psi}_c \star \cdots \star \widetilde{\psi}_f,$$

with $2N$ generators $\widetilde{\psi}_a, \cdots, \widetilde{\psi}_f$. In the first step we eliminate $\widetilde{\psi}_a$ from the expectation value by a pull through formula. To this end we use $\{\widetilde{\psi}_a, \widetilde{\psi}_b\}_\star := \widetilde{\psi}_a \star \widetilde{\psi}_b + \widetilde{\psi}_b \star \widetilde{\psi}_a$ which is either 1, -1 or 0. This yields

$$\begin{aligned}
&\left\langle \widetilde{\psi}_a \star \widetilde{\psi}_b \star \widetilde{\psi}_c \star \cdots \star \widetilde{\psi}_f \right\rangle_{\varkappa_\mu} \\
&\quad = \{\widetilde{\psi}_a, \widetilde{\psi}_b\}_\star \left\langle \widetilde{\psi}_c \star \widetilde{\psi}_d \star \cdots \star \widetilde{\psi}_f \right\rangle_{\varkappa_\mu} - \{\widetilde{\psi}_a, \widetilde{\psi}_c\}_\star \left\langle \widetilde{\psi}_b \star \widetilde{\psi}_d \star \cdots \star \widetilde{\psi}_f \right\rangle_{\varkappa_\mu} \\
&\qquad + \{\widetilde{\psi}_a, \widetilde{\psi}_d\}_\star \left\langle \widetilde{\psi}_b \star \widetilde{\psi}_c \star \cdots \star \widetilde{\psi}_f \right\rangle_{\varkappa_\mu} + \ldots \\
&\qquad + \left\{\widetilde{\psi}_a, \widetilde{\psi}_f\right\}_\star \langle \widetilde{\psi}_b \star \widetilde{\psi}_c \star \cdots \star \widetilde{\psi}_e \rangle_{\varkappa_\mu} - \left\langle \widetilde{\psi}_b \star \widetilde{\psi}_c \star \cdots \star \widetilde{\psi}_f \star \widetilde{\psi}_a \right\rangle_{\varkappa_\mu}.
\end{aligned}$$

Afterwards we use the cyclicity of the Grassmann integral in the last expectation value on the r.h.s. of the latter expression and the identities

$$\overline{\psi}_i \star \varkappa_\mu = \mathrm{e}^{q_i}\, \varkappa_\mu \star \overline{\psi}_i \quad \text{and} \quad \psi_i \star \varkappa_\mu = \mathrm{e}^{-q_i}\, \varkappa_\mu \star \psi_i$$

which follow from the fact that $\varkappa_\mu$ is a star product of single states of the form $r_i \overline{\psi}_i \psi_i + 1$ and the CAR for the star product. Thus, the last expectation value can be written as

$$\left\langle \widetilde{\psi}_b \star \widetilde{\psi}_c \star \cdots \star \widetilde{\psi}_f \star \widetilde{\psi}_a \right\rangle_{\varkappa_\mu} = \mathrm{e}^{\pm q_a} \left\langle \widetilde{\psi}_a \star \widetilde{\psi}_b \star \widetilde{\psi}_c \star \cdots \star \widetilde{\psi}_f \right\rangle_{\varkappa_\mu}$$

and we conclude with

$$\begin{aligned}
&\left\langle \widetilde{\psi}_a \star \widetilde{\psi}_b \star \widetilde{\psi}_c \star \cdots \star \widetilde{\psi}_f \right\rangle_{\varkappa_\mu} \\
&\quad = \frac{\{\widetilde{\psi}_a, \widetilde{\psi}_b\}_\star}{1 + \mathrm{e}^{\pm q_a}} \left\langle \widetilde{\psi}_c \star \widetilde{\psi}_d \star \cdots \star \widetilde{\psi}_f \right\rangle_{\varkappa_\mu} - \frac{\{\widetilde{\psi}_a, \widetilde{\psi}_c\}_\star}{1 + \mathrm{e}^{\pm q_a}} \left\langle \widetilde{\psi}_b \star \widetilde{\psi}_d \star \cdots \star \widetilde{\psi}_f \right\rangle_{\varkappa_\mu} \\
&\qquad + \frac{\{\widetilde{\psi}_a, \widetilde{\psi}_d\}_\star}{1 + \mathrm{e}^{\pm q_a}} \left\langle \widetilde{\psi}_b \star \widetilde{\psi}_c \star \cdots \star \widetilde{\psi}_f \right\rangle_{\varkappa_\mu} + \ldots \\
&\qquad + \frac{\left\{\widetilde{\psi}_a, \widetilde{\psi}_f\right\}_\star}{1 + \mathrm{e}^{\pm q_a}} \langle \widetilde{\psi}_b \star \widetilde{\psi}_c \star \cdots \star \widetilde{\psi}_e \rangle_{\varkappa_\mu}.
\end{aligned}$$

We have reduced the expectation value of $2N$ generators to a sum of expectation values of $2(N-1)$ generators. As in [Gau60] the assertion follows by an induction in the number of generators. Finally the quasifreeness of $\varkappa$ follows from

$$\varkappa = \lim_{\mu \to \infty} \frac{\varkappa_\mu}{\int \mathcal{D}(\overline{\Psi}, \Psi) \varkappa_\mu}$$

which completes the proof. □

Remark 5.50. Carrying out the $|M|$-fold star product in $\varkappa_\mu$, we find a more convenient form of $\varkappa_\mu$:

$$\varkappa_\mu = \sum_{Q \subseteq M} (-1)^{s_Q} \prod_{i \in Q} r_i \prod_{i \in Q} \overline{\psi}_i \prod_{i \in Q} \psi_i = \sum_{Q \subseteq M} (-1)^{s_Q} r_Q \overline{\Psi}_Q \Psi_Q$$

where $s_Q := \frac{1}{2}|Q|(|Q|-1)$, $r_Q := \prod_{i \in Q} r_i$. The sum runs over all ordered subsets $Q \subseteq M$.

Appendix **A**

Generalized Two-Particle Density Matrix as 7×7-Matrix

In this appendix we give a more explicit, basis dependent form of the generalized 2-particle density matrix $\widehat{\Gamma}$. We assume $\{\phi_k\}_{k=1}^{\infty}$ to be a fixed, but arbitrary ONB of $\mathfrak{h}$. Recall that $\widehat{\Gamma}$ is defined as a 7×7-matrix on $\mathcal{H}_{\mathrm{sim}}$ in Definition 3.29. In order to simplify notation, it is convenient to define some operators and functionals.

Definition A.1. Let $f_1, f_2, g_1, g_2, f, g \in \mathfrak{h}$, and $\mu \in \mathbb{C}$. We define $\mathcal{D}(B) := \left\{F \in \mathfrak{h} \otimes \mathfrak{h} \middle| \sum_{k=1}^{\infty} \langle \phi_k \otimes \phi_k, F \rangle_{\mathfrak{h}\otimes\mathfrak{h}} < \infty \right\} \subseteq \mathfrak{h} \otimes \mathfrak{h}$ and the following linear maps:

$$\Lambda_1 : \mathfrak{h} \otimes \mathfrak{h} \to \mathfrak{h} \otimes \mathfrak{h},$$
$$\langle g_1 \otimes g_2, \Lambda_1 (f_1 \otimes f_2) \rangle := \omega\big(a^*(f_1)\, a^*(f_2)\, a^*(\overline{g}_2)\, a(g_1)\big),$$
$$\Lambda_2^* : \mathfrak{h} \otimes \mathfrak{h} \to \mathfrak{h} \otimes \mathfrak{h},$$
$$\langle g_1 \otimes g_2, \Lambda_2^* (f_1 \otimes f_2) \rangle := \omega\big(a^*(f_1)\, a^*(f_2)\, a^*(\overline{g}_2)\, a^*(\overline{g}_1)\big),$$
$$\Delta : \mathfrak{h} \otimes \mathfrak{h} \to \mathfrak{h} \otimes \mathfrak{h},\ \langle g_1 \otimes g_2, \Delta (f_1 \otimes f_2) \rangle := \omega\big(a^*(f_1)\, a^*(\overline{g}_1)\, a(g_2)\, a(\overline{f}_2)\big),$$
$$A_1 : \mathfrak{h} \otimes \mathfrak{h} \to \mathfrak{h},\ \langle g, A_1 (f_1 \otimes f_2) \rangle := \omega\big(a^*(f_1)\, a^*(f_2)\, a(g)\big),$$
$$A_2^* : \mathfrak{h} \otimes \mathfrak{h} \to \mathfrak{h},\ \langle g, A_2^* (f_1 \otimes f_2) \rangle := \omega\big(a^*(f_1)\, a^*(f_2)\, a^*(\overline{g})\big),$$
$$Q_1 : \mathfrak{h} \otimes \mathfrak{h} \to \mathfrak{h},\ \langle g, Q_1 (f_1 \otimes f_2) \rangle := \omega\big(a^*(f_1)\, a(\overline{f}_2)\, a(g)\big),$$
$$Q_2 : \mathfrak{h} \otimes \mathfrak{h} \to \mathfrak{h},\ \langle g, Q_2 (f_1 \otimes f_2) \rangle := \omega\big(a^*(f_1)\, a(\overline{f}_2)\, a^*(\overline{g})\big),$$
$$B : \mathcal{D}(B) \to \mathfrak{h} \otimes \mathfrak{h},\ B := \sum_{i,k=1}^{\infty} |\phi_i \otimes \phi_i\rangle \langle \phi_k \otimes \phi_k| ,$$
$$\beta_2 : \mathbb{C} \otimes \mathfrak{h} \to \mathfrak{h},\ \beta_2 := \sum_{i=1}^{\infty} |\phi_i\rangle \langle 1 \otimes \phi_i| ,$$
$$\beta_1 : \mathcal{D}(B) \to \mathbb{C},\ \beta_1 := \sum_{i=1}^{\infty} \langle \phi_i \otimes \phi_i| .$$

Furthermore, recall from Remark 3.26 that b is given by $\langle b, f \rangle_{\mathfrak{h}} := \omega\left(a^*(f)\right)$. As we already pointed out in Proposition 3.30, the generalized

2-pdm is selfadjoint. Since therefore $\widehat{\Gamma}_{ij} = \overline{\widehat{\Gamma}}_{ji}$, it suffices to state the entries $\widehat{\Gamma}_{ij}$ for $1 \leq i \leq j \leq 7$. Using the notation specified before and $\mathbb{1} \equiv \mathbb{1}_{\mathfrak{h}}$, we have:

$$\widehat{\Gamma}_{11} = \Gamma : \mathfrak{h} \otimes \mathfrak{h} \to \mathfrak{h} \otimes \mathfrak{h},$$
$$\widehat{\Gamma}_{12} = \Lambda_1^* : \mathfrak{h} \otimes \mathfrak{h} \to \mathfrak{h} \otimes \mathfrak{h},$$
$$\widehat{\Gamma}_{13} = \Lambda_1^* \mathrm{Ex} + (\alpha \otimes \mathbb{1})\, B : \mathfrak{h} \otimes \mathfrak{h} \to \mathfrak{h} \otimes \mathfrak{h},$$
$$\widehat{\Gamma}_{14} = \Lambda_2 : \mathfrak{h} \otimes \mathfrak{h} \to \mathfrak{h} \otimes \mathfrak{h},$$
$$\widehat{\Gamma}_{15} = A_1^* : \mathfrak{h} \to \mathfrak{h} \otimes \mathfrak{h},$$
$$\widehat{\Gamma}_{16} = A_2 : \mathfrak{h} \to \mathfrak{h} \otimes \mathfrak{h},$$
$$\widehat{\Gamma}_{17} = (\alpha \otimes \mathbb{1})\, \beta_1^* : \mathbb{C} \to \mathfrak{h} \otimes \mathfrak{h},$$
$$\widehat{\Gamma}_{22} = \mathrm{Ex}\Delta + \gamma \otimes \mathbb{1} : \mathfrak{h} \otimes \mathfrak{h} \to \mathfrak{h} \otimes \mathfrak{h},$$
$$\widehat{\Gamma}_{23} = \Delta^* + (\gamma \otimes \mathbb{1})\,(B + \mathrm{Ex}) : \mathfrak{h} \otimes \mathfrak{h} \to \mathfrak{h} \otimes \mathfrak{h},$$
$$\widehat{\Gamma}_{24} = \mathrm{Ex}\overline{\Lambda}_1 + (\alpha \otimes \mathbb{1})\,(\mathbb{1}_{\mathfrak{h}\otimes\mathfrak{h}} + \mathrm{Ex}) : \mathfrak{h} \otimes \mathfrak{h} \to \mathfrak{h} \otimes \mathfrak{h},$$
$$\widehat{\Gamma}_{25} = Q_1^* : \mathfrak{h} \to \mathfrak{h} \otimes \mathfrak{h},$$
$$\widehat{\Gamma}_{26} = Q_2^* : \mathfrak{h} \to \mathfrak{h} \otimes \mathfrak{h},$$
$$\widehat{\Gamma}_{27} = (\mathbb{1} \otimes \gamma)\, \beta_1^* : \mathbb{C} \to \mathfrak{h} \otimes \mathfrak{h},$$
$$\widehat{\Gamma}_{33} = \Delta\mathrm{Ex} + (\mathbb{1} \otimes \gamma)\, B + B\,(\mathbb{1} \otimes \gamma) + B + \mathbb{1} \otimes \gamma : \mathfrak{h} \otimes \mathfrak{h} \to \mathfrak{h} \otimes \mathfrak{h},$$
$$\widehat{\Gamma}_{34} = \overline{\Lambda}_1 + (\mathbb{1} \otimes \alpha)\,(\mathbb{1}_{\mathfrak{h}\otimes\mathfrak{h}} + \mathrm{Ex}) + B\,(\mathbb{1} \otimes \alpha) : \mathfrak{h} \otimes \mathfrak{h} \to \mathfrak{h} \otimes \mathfrak{h},$$
$$\widehat{\Gamma}_{35} = \mathrm{Ex}Q_1^* + \beta_1^* b^* : \mathfrak{h} \to \mathfrak{h} \otimes \mathfrak{h},$$
$$\widehat{\Gamma}_{36} = \mathrm{Ex}Q_2^* + \beta_1^* \overline{b}^* : \mathfrak{h} \to \mathfrak{h} \otimes \mathfrak{h},$$
$$\widehat{\Gamma}_{37} = (\mathbb{1} \otimes \mathbb{1} + \mathbb{1} \otimes \gamma)\, \beta_1^* : \mathbb{C} \to \mathfrak{h} \otimes \mathfrak{h},$$
$$\widehat{\Gamma}_{44} = \Gamma^T + (\mathbb{1} \otimes \mathbb{1} + \overline{\gamma} \otimes \mathbb{1} + \mathbb{1} \otimes \overline{\gamma})\,(\mathbb{1}_{\mathfrak{h}\otimes\mathfrak{h}} + \mathrm{Ex}) : \mathfrak{h} \otimes \mathfrak{h} \to \mathfrak{h} \otimes \mathfrak{h},$$
$$\widehat{\Gamma}_{45} = \overline{A}_2 : \mathfrak{h} \to \mathfrak{h} \otimes \mathfrak{h},$$
$$\widehat{\Gamma}_{46} = \overline{A}_1^* + (\mathbb{1}_{\mathfrak{h}\otimes\mathfrak{h}} + \mathrm{Ex})\,(\mathbb{1} \otimes b)\, \beta_2^* : \mathfrak{h} \to \mathfrak{h} \otimes \mathfrak{h},$$
$$\widehat{\Gamma}_{47} = (\alpha^* \otimes \mathbb{1})\, \beta_1^* : \mathbb{C} \to \mathfrak{h} \otimes \mathfrak{h},$$
$$\widehat{\Gamma}_{55} = \gamma : \mathfrak{h} \to \mathfrak{h},$$
$$\widehat{\Gamma}_{56} = \alpha : \mathfrak{h} \to \mathfrak{h},$$
$$\widehat{\Gamma}_{57} = b : \mathbb{C} \to \mathfrak{h},$$
$$\widehat{\Gamma}_{66} = \mathbb{1} + \overline{\gamma} : \mathfrak{h} \to \mathfrak{h},$$
$$\widehat{\Gamma}_{67} = \overline{b} : \mathbb{C} \to \mathfrak{h},$$
$$\widehat{\Gamma}_{77} = 1 : \mathbb{C} \to \mathbb{C}.$$

Remark A.2. Both generalizations of the 1-pdm, given in Definitions 3.21 and 3.25, are contained in the generalized 2-pdm, namely

$$\widetilde{\gamma} = \begin{pmatrix} \widehat{\Gamma}_{55} & \widehat{\Gamma}_{65} \\ \widehat{\Gamma}_{56} & \widehat{\Gamma}_{66} \end{pmatrix} \quad \text{and} \quad \widehat{\gamma} = \begin{pmatrix} \widehat{\Gamma}_{55} & \widehat{\Gamma}_{65} & \widehat{\Gamma}_{75} \\ \widehat{\Gamma}_{56} & \widehat{\Gamma}_{66} & \widehat{\Gamma}_{76} \\ \widehat{\Gamma}_{57} & \widehat{\Gamma}_{67} & \widehat{\Gamma}_{77} \end{pmatrix}.$$

Appendix **B**

Diagonalization of Selfadjoint Polynomials of Degree 2 for Bosons

For bosons we show that certain polynomials of degree 2 in creation and annihilation operators can be unitarily transformed into a polynomial of a simpler form. Before stating and proving the assertion we specify the notation. If $\mathcal{P}$ is a selfadjoint polynomial in creation and annihilation operators, there are an ONB $\{\varphi_k\}_{k=1}^{\infty}$ of $\mathfrak{h}$, $N \in \mathbb{N}$, $\mu \in \mathbb{R}$, and coefficients $\kappa_{kl}, \lambda_{kl}, \eta_k \in \mathbb{C}$ with $\lambda_{lk} = \lambda_{kl}$, $\overline{\kappa}_{lk} = \kappa_{kl}$, such that

$$\mathcal{P} = \sum_{k,l=1}^{N} \left(\lambda_{kl} a_k^* a_l^* + \kappa_{kl} a_k^* a_l + \overline{\lambda}_{lk} a_k a_l \right) + \sum_{k=1}^{N} \left(\overline{\eta}_k a_k + \eta_k a_k^* \right) + \mu.$$

We define two complex $N \times N$-matrices K and L by $K_{kl} := \kappa_{kl}$ and $L_{kl} := 2\lambda_{kl}$, respectively. Note that K is selfadjoint while in general $L = L^T$. Using $\vec{a} := \left(a_1, \ldots, a_N, a_1^*, \ldots, a_N^*\right)^T$ as an operator on $(\mathcal{F}^+)^{\otimes 2N}$, we can rewrite $\mathcal{P}$ in the compact form

$$\mathcal{P} = \frac{1}{2} \left(\, \vec{a} \, \middle| \, M\vec{a} \, \right) + \left(\, \vec{\eta} \, \middle| \, \vec{a} \, \right) + \widetilde{\mu}$$

with $M := \begin{pmatrix} K & L \\ L^* & K^T \end{pmatrix} \in \mathbb{C}^{2N \times 2N}$, $\vec{\eta} := \left(\eta_1, \ldots, \eta_N, \overline{\eta}_1, \ldots, \overline{\eta}_N\right)^T \in \mathbb{C}^{2N}$, and $\widetilde{\mu} := \mu - \frac{1}{2} \mathrm{tr}\,(K)$. Here

$$(\,\cdot\,|\,\cdot\,) : \left(\mathcal{A}^+\right)^{2N} \times \left(\mathcal{A}^+\right)^{2N} \to \mathcal{A}^+, \ \left(\vec{x} \middle| \vec{y}\right) := \sum_{k=1}^{2N} x_k^* y_k.$$

Lemma B.1. *Let $\mathcal{P}$ be a selfadjoint polynomial of degree 2 in creation and annihilation operators and $\{\varphi_k\}_{k=1}^{\infty}$ an ONB of $\mathfrak{h}$ such that, using the notation specified above,*

$$\mathcal{P} = \frac{1}{2} \left(\, \vec{a} \, \middle| \, M\vec{a} \, \right) + \left(\, \vec{\eta} \, \middle| \, \vec{a} \, \right) + \widetilde{\mu}$$

with $M := \begin{pmatrix} K & L \\ L^* & K^T \end{pmatrix} \in \mathbb{C}^{2N\times 2N}$, $K^* = \overline{K} = K$, $L^T = \overline{L} = L$, $\vec{\eta} := (\eta_1, \ldots, \eta_N, \overline{\eta_1}, \ldots, \overline{\eta_N})^T \in \mathbb{C}^{2N}$, *and* $\widetilde{\mu} \in \mathbb{R}$. *Moreover, we assume that there is a constant* $c > 0$ *such that* $K + L \geq c\mathbb{1}$ *and* $K - L \geq c\mathbb{1}$. *Then, there is a unitary transformation which maps* $\mathcal{P}$ *to a selfadjoint polynomial of the form*

$$\widetilde{\mathcal{P}} = \widehat{\mathbb{E}} + a^*(\tau) + a(\tau) + \nu, \tag{B.1}$$

where $\nu \in \mathbb{R}$, $\widehat{\mathbb{E}}$ *is the second quantization of a selfadjoint one-particle operator* E, *and* $\tau \in \operatorname{ran}(E)^\perp \subseteq \mathfrak{h}$.

The proof is a generalization of [Ber66, Section 8] and [BR86, Chapter 3], where polynomials are considered which have a term quadratic in creation and annihilation operators (and a constant term in [BR86]), but no terms linear in creation and annihilation operators.

Proof. First, we diagonalize the matrix M and refer to [Ber66] for this step. Afterwards, we use a Weyl transformation to cancel, at least partially, terms linear in creation and annihilation operators. Finally, we merge the remaining terms.

Theorem 8.1 of [Ber66] states that, under the conditions specified in the lemma, a purely quadratic selfadjoint polynomial can be transformed by a (unitary implementable) Bogoliubov map U into $\sum_{k,l=1}^N \widetilde{\kappa}_{kl} a_k^* a_l + \widetilde{\nu}$ with $\widetilde{\nu} \in \mathbb{C}$ and matrix elements $\widetilde{\kappa}_{kl}$ of a selfadjoint one-particle operator $\widetilde{K}$. Without loss of generality, we may assume that $\widetilde{K}$ is diagonal in the given basis, since, for a given basis, any selfadjoint matrix can be unitarily transformed into an operator diagonal in this basis. Denoting $b_k^* := \mathbb{U}_U a_k^* \mathbb{U}_U^*$ and, consequently, $b_k = \mathbb{U}_U a_k \mathbb{U}_U^*$ for any $k = 1, \ldots, N$, we therefore have

$$\mathbb{U}_U \mathcal{P} \mathbb{U}_U^* = \sum_{k=1}^N \left(\epsilon_k b_k^* b_k + \eta_k b_k^* + \overline{\eta}_k b_k \right) + (\widetilde{\nu} + \widetilde{\mu}) \,.$$

Using the linearity of the creation operators and the antilinearity of the annihilation operators, we can rewrite the linear part as

$$\sum_{k=1}^N \left(\eta_k b_k^* + \overline{\eta}_k b_k \right) = b^*(\eta) + b(\eta),$$

where $\eta := \sum_{k=1}^N \eta_k \varphi_k \in \mathfrak{h}$, $b^*(\eta) := \mathbb{U}_U a^*(\eta) \mathbb{U}_U^*$ and $b(\eta) := \mathbb{U}_U a(\eta) \mathbb{U}_U^*$. Furthermore, the quadratic part can be considered as the second quantization $\widehat{\mathbb{E}}$ of a selfadjoint one-particle operator E with $\langle \varphi_k, E\varphi_k \rangle_{\mathfrak{h}} = \epsilon_k$, $k \in \mathbb{N}$, and, therefore,

$$\mathbb{U}_U \mathcal{P} \mathbb{U}_U^* = \widehat{\mathbb{E}} + (b^*(\eta) + b(\eta)) + (\widetilde{\nu} + \widetilde{\mu}) \,.$$

The operator E is related to K and L via $U^* \begin{pmatrix} K & L \\ L^* & K^T \end{pmatrix} U = \begin{pmatrix} E & 0 \\ 0 & E^T \end{pmatrix}$.

In the next step, we take care of the terms linear in creation and annihilation operators. To this purpose, we apply a Weyl transformation given by $\mathbb{W}_{-f}$ with $f \in \operatorname{span}\{\varphi_k\}_{k=1}^N \subseteq \mathfrak{h}$ to the polynomial. In the following computation, we determine the specific choice of f to cancel part of the linear terms. Since $\mathbb{W}_{-f} b_k \mathbb{W}_{-f}^* = b_k - \langle \varphi_k, f \rangle_{\mathfrak{h}}$ and $\mathbb{W}_{-f} b_k^* \mathbb{W}_{-f}^* = b_k^* - \langle f, \varphi_k \rangle_{\mathfrak{h}}$, we obtain

$$\begin{aligned}\mathbb{W}_{-f}\mathbb{U}_U \mathcal{P} \mathbb{U}_U^* \mathbb{W}_{-f}^* = \sum_{k=1}^{N} \Big[&\epsilon_k b_k^* b_k - \epsilon_k \left(\langle f, \varphi_k \rangle_{\mathfrak{h}} b_k - \langle \varphi_k, f \rangle_{\mathfrak{h}} b_k^* \right) \\ &+ \epsilon_k \langle f, \varphi_k \rangle_{\mathfrak{h}} \langle \varphi_k, f \rangle_{\mathfrak{h}} + (\eta_k b_k^* + \overline{\eta}_k b_k) \\ &- \left(\eta_k \langle f, \varphi_k \rangle_{\mathfrak{h}} + \overline{\eta}_k \langle \varphi_k, f \rangle_{\mathfrak{h}} \right) \Big] + (\widetilde{\nu} + \widetilde{\mu})\end{aligned}$$

and, with the notation as above,

$$\begin{aligned}\mathbb{W}_{-f}\mathbb{U}_U \mathcal{P} \mathbb{U}_U^* \mathbb{W}_{-f}^* &= \widehat{\mathbb{E}} + (b^*(-Ef + \eta) + b(-Ef + \eta)) \\ &+ \left(\langle f, Ef \rangle_{\mathfrak{h}} - \langle f, \eta \rangle_{\mathfrak{h}} - \langle \eta, f \rangle_{\mathfrak{h}} + \widetilde{\nu} + \widetilde{\mu} \right).\end{aligned}$$

We decompose the vector $\eta \in \mathfrak{h}$ to obtain the linear part of (B.1). Therefore, we denote by $\mathcal{P}$ the orthogonal projection on $\operatorname{ran}(E) \subseteq \mathfrak{h}$ and by $\mathcal{P}^\perp$ the orthogonal projection on $\operatorname{ran}(E)^\perp \subseteq \mathfrak{h}$. Then, we write

$$\eta = \zeta + \tau,$$

where $\zeta := \mathcal{P}\eta \in \operatorname{ran}(E)$ and $\tau := \mathcal{P}^\perp \eta \in \operatorname{ran}(E)^\perp$. Thus,

$$b^*(-Ef + \eta) + b(-Ef + \eta) = b^*(-Ef + \zeta) + b(-Ef + \zeta) + b^*(\tau) + b(\tau). \tag{B.2}$$

Since $\zeta \in \operatorname{ran}(E)$, there is a $f \in \mathfrak{h}$ such that $Ef = \zeta$. Choosing this f as the parameter of the Weyl transformation, the first two terms on the right hand side of Equation (B.2) vanish and the other two terms yield the asserted linear part of Equation (B.1).

Finally, we note that the two terms $\langle f, \eta \rangle_{\mathfrak{h}} + \langle \eta, f \rangle_{\mathfrak{h}} = 2\operatorname{Re}\left(\langle \eta, f \rangle_{\mathfrak{h}} \right)$ and, since E is selfadjoint, $\langle f, Ef \rangle_{\mathfrak{h}}$ are real numbers. Thus, if we set $\nu := \langle f, Ef \rangle_{\mathfrak{h}} - 2\operatorname{Re}\left(\langle \eta, f \rangle_{\mathfrak{h}} \right) + \widetilde{\nu} + \widetilde{\mu}$, $\widetilde{\mathcal{P}} := \mathbb{W}_{-f}\mathbb{U}_U \mathcal{P} \mathbb{U}_U^* \mathbb{W}_{-f}^*$ is of the asserted form. □

Bibliography

[Ara71] H. Araki, *On Quasifree States of CAR and Bogoliubov Automorphisms*, Publications RIMS Kyoto University **6** (1970/71), 385–442.

[Bac91] V. Bach, *Ionization Energies of Bosonic Coulomb Systems*, Letters in Mathematical Physics **21** (1991), 139–149.

[Bac92] ______, *Error Bound for the Hartree–Fock Energy of Atoms and Molecules*, Communications in Mathematical Physics **147** (1992), 527–548.

[Bac93] ______, *Accuracy of Mean Field Approximations for Atoms and Molecules*, Communications in Mathematical Physics **155** (1993), 295–310.

[BBKM13] V. Bach, S. Bréteaux, H. K. Knörr, and E. Menge, *Generalized One-Particle Density Matrices and Quasifree States*, Preprint arXiv:1304.7995 (2013).

[BBT13] V. Bach, S. Bréteaux, and T. Tzaneteas, *Minimization of the Energy of the Non-Relativistic One-Electron Pauli–Fierz Model over Quasifree States*, Preprint arXiv:1301.0936 (2013).

[Ber66] F. A. Berezin, *The Method of Second Quantization*, Academic Press, New York, London, 1966.

[BKM12] V. Bach, H. K. Knörr, and E. Menge, *Fermion Correlation Inequalities derived from G- and P-Conditions*, Documenta Mathematica **17** (2012), 451–481.

[BKM13] ______, *Representability Conditions by Grassmann Integration*, Preprint arXiv:1307.0465 (2013).

[BLS94] V. Bach, E. H. Lieb, and J. P. Solovej, *Generalized Hartree–Fock Theory and the Hubbard Model*, Journal of Statistical Physics **76** (1994), no. 1/2, 3–89.

[BR79] O. Bratteli and D. W. Robinson, *Operator Algebras and Quantum Statistical Mechanics I – C^* and W^*-Algebras, Symmerty Groups, Decomposition of States*, Texts and Monographs in Physics, Springer-Verlag, New York, Heidelberg, Berlin, 1979.

[BR81] ______, *Operator Algebras and Quantum Statistical Mechanics II – Equilibrium States, Models in Quantum Statistical Mechanics*, Texts and Monographs in Physics, Springer-Verlag, New York, Heidelberg, Berlin, 1981.

[BR86] J.-P. Blaizot and G. Ripka, *Quantum Theory of Finite Systems*, MIT Press, Cambridge (Mass.), London (England), 1986.

[CLS06] E. Cancés, M. Lewin, and G. Stoltz, *The electornic ground state energy problem: A new reduced density matrix approach*, The Journal of Chemical Physics **125** (2006), 064101.

[Col63] A. J. Coleman, *Structure of Fermion Density Matrices*, Reviews of Modern Physics **35** (1963), no. 3, 668–687, Discussion pp. 687–689.

[CR12] M. Combescure and D. Robert, *Coherent States and Applications in Mathematical Physics*, Theoretical and Mathematical Physics, Springer-Verlag, Dordrecht, Heidelberg, London, New York, 2012.

[DL67] F. J. Dyson and A. Lenard, *Stability of Matter. I*, Journal of Mathematical Physics **8** (1967), no. 3, 423–434.

[dSP05] W. d. S. Pedra, *Zur mathematischen Theorie der Fermiflüssigkeiten bei positiven Temperaturen*, Ph.D. thesis, Universität Leipzig, 2005.

[Dys67] F. J. Dyson, *Ground-State Energy of a Finite System of Charged Particles*, Journal of Mathematical Physics **8** (1967), no. 8, 1538–1545.

[Erd78a] R. M. Erdahl, *On the Structure of the Diagonal Conditions*, International Journal of Quantum Chemistry **13** (1978), no. 6, 731–736.

[Erd78b] ______, *Representability*, International Journal of Quantum Chemistry **13** (1978), no. 6, 697–718.

[FdlL86] C. Fefferman and R. de la Llave, *Relativistic Stability of Matter – I*, Revista Mathemática Iberoamericana **2** (1986), no. 1/2, 119–160.

[FKT02] J. Feldman, H. Knörrer, and E. Trubowitz, *Fermionic Functional Integrals and the Renormalization Group*, CRM Monograph Series, vol. 16, American Mathematical Society, Providence (R.I.), 2002.

[Gau60] M. Gaudin, *Une Démonstation Simplifiée du Théorème de Wick en Méchanique Statistique*, Nuclear Physics **15** (1960), 89–91.

[GM04] G. Gidofalvi and D. A. Mazziotti, *Boson correlation energies via variational minimization with the two-particle reduced density matrix: Exact N-representability conditions for harmonic interactions*, Physical Review A **69** (2004), 042511.

[GP64] C. Garrod and J. K. Percus, *Reduction of the N-Particle Variational Problem*, Journal of Mathematical Physics **5** (1964), no. 12, 1756–1776.

[GS94] G. M. Graf and J. P. Solovej, *A correlation estimate with applications to quantum systems with Coulomb interactions*, Reviews in Mathematical Physics **6** (1994), no. 5a (Special Issue), 977–997.

[HS02] C. Hainzl and R. Seiringer, *General Decomposition of Radial Functions on $\mathbb{R}^n$ and Applications to N-Body Quantum Systems*, Letters in Mathematical Physics **61** (2002), 75–84.

[LD68] A. Lenard and F. J. Dyson, *Stability of Matter. II*, Journal of Mathematical Physics **9** (1968), no. 5, 698–711.

[Lie81] E. H. Lieb, *Variational Principle for Many-Fermion Systems*, Physical Review Letters **46** (1981), no. 7, 457–459.

[Löw55] P.-O. Löwdin, *Quantum Theory of Many-Particle Systems. I. Physical Interpretations by Means of Density Matrices, Natural Spin-Orbitals, and Convergence Problems in the Method of Configurational Interaction*, Physical Review **97** (1955), no. 6, 1474–1489.

[LS04] E. H. Lieb and J. P. Solovej, *Ground State Energy of the Two-Component Bose Gas*, Communications in Mathematical Physics **252** (2004), 485–534.

[LS10] E. H. Lieb and R. Seiringer, *The Stability of Matter in Quantum Mechanics*, Cambridge University Press, Cambridge (UK), 2010.

[LSSY05] E. H. Lieb, R. Seiringer, J. P. Solovej, and J. Yngvason, *The Mathematics of the Bose Gas and its Condensation*, Oberwolfach Seminars, vol. 34, Birkhäuser, Basel, 2005.

[LT75] E. H. Lieb and W. Thirring, *Bound for the Kinetic Energy of Fermions Which Proves the Stability of Matter*, Physical Review Letters **35** (1975), no. 11, 687–689, (Erratum **35** (1975), no. 16, 1116).

[LY98] E. H. Lieb and J. Yngvason, *Ground State Energy of the Low Density Bose Gas*, Physical Review Letters **80** (1998), no. 12, 2504–2507.

[Maz02] D. A. Mazziotti, *Variational minimization of atomic and molecular ground-state energies via the two-particle reduced density matrix*, Physical Review A **65** (2002), 062511.

[Maz12a] ______, *Significant conditions for the two-electron reduced density matrix from the constructive solution of N representability*, Physical Review A **85** (2012), 062507.

[Maz12b] ———, *Structure of Fermionic Density Matrices: Complete N-representability Conditions*, Physical Review Letters **108** (2012), 263002.

[ME01] D. A. Mazziotti and R. M. Erdahl, *Uncertainty relations and reduced density matrices: Mapping many-body quantum mechanics onto four particles*, Physical Review A **63** (2001), 042113.

[NAHM11] K. Naftchi-Ardebili, N. W. Hau, and D. A. Mazziotti, *Rank restriction for the variational calculation of two-electron reduced density matrices of many-electron atoms and molecules*, Physical Review A **84** (2011), 052506.

[Nam11] P. T. Nam, *Contributions to the rigorous study of the structure of atoms*, Ph.D. thesis, University of Copenhagen, 2011, (Paper III. Bogoliubov theory and bosonic atoms, Preprint arXiv:1109.2875).

[Ray78] J. W. Strutt, 3rd Baron Rayleigh, *Theory of Sound*, vol. I and II, Macmillan, London, 1877/78.

[Rit09a] W. Ritz, *Theorie der Transversalschwingungen einer quadratischen Platte mit freien Rändern*, Annalen der Physik **333** (1909), 737–786.

[Rit09b] ———, *Über eine neue Methode zur Lösung gewisser Variationsprobleme der mathematischen Physik*, Journal für reine und angewandte Mathematik **135** (1909), 1–61.

[RSSS12] V. Rivasseau, R. Seiringer, J. P. Solovej, and T. Spencer, *Quantum many body systems. Cetraro, Italy 2010. Selected papers based on the presentations at the CIME school, August 30 to September 4, 2010.*, Lecture Notes in Mathematics - CIME Foundation Subseries, vol. 2051, Springer-Verlag, Berlin, 2012.

[Sal98] M. Salmhofer, *Renormalization — An Introduction*, Springer-Verlag, Berlin, Heidelberg, 1998.

[Sol06] J. P. Solovej, *Upper Bounds to the Ground State Energies of the One- and Two-Component Charged Bose Gases*, Communications in Mathematical Physics **266** (2006), 797–818.

[Sol07] ———, *Many Body Quantum Mechanics*, Lecture Notes, 2007.

[SS65] D. Shale and W. F. Stinespring, *Spinor Representation of Infinite Orthogonal Groups*, Journal of Mathematics and Mechanics **14** (1965), no. 2, 315–322.

[Tak08] L. A. Takhtajan, *Quantum Mechanics for Mathematicians*, Graduate Studies in Mathematics, vol. 95, American Mathematical Society, Providence (R.I.), 2008.

[Thi08] W. Thirring, *Quantenmechanik großer Systeme*, Lehrbuch der Mathematischen Physik, vol. 4, Springer-Verlag, Wien, 2008.

[ZB01] V. A. Zagrebnov and J.-B. Bru, *The Bogoliubov model of weakly imperfect Bose gas*, Physical Reports **350** (2001), 291–434.

[ZBF+04] Z. Zhao, B. J. Braams, M. Fukuda, M. L. Overton, and J. K. Percus, *The reduced density matrix method for electronic structure calculations and the role of three-index representability conditions*, Journal of Chemical Physics **120** (2004), no. 5, 2095–2104.