First-Order Corrections to the Mean-Field Limit and Quantum Walks with Non-Orthogonal Position States

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Abstract

Many-particle quantum systems are a fundamental research area in quantum physics. For example, they provide the microscopic description of macroscopic solid-state systems, like magnets or superconductors, and it is desired to derive macroscopically observable phenomena like para- or ferromagnetism or superconductivity from the microscopic description. However, already computing the ground-state energy of such systems is computationally hard in general, in some cases even for quantum computers. Therefore, researchers largely rely on different approximation methods, one of the most common being mean-field theory. Despite its extensive usage, general methods to estimate the quality of this approximation do not exist.

In the first part of this thesis, we develop an algebraic theory for the first-order corrections to the mean-field limit for a class of mean-field models introduced by Raggio and Werner in 1989. We use a concept called fluctuations, which has been previously used in translationally invariant systems in the sense of a non-commutative central limit theorem and has been applied to mean-field models in a basic manner before. We show that in the context of mean-field models they give rise to an algebra of canonical commutation relations, which conveniently quantifies the first-order asymptotics and can be understood as an asymptotic extension beyond variation over product states. We present the detailed structure of the fluctuation algebra and identify the related normal modes. Based on this, we develop an estimation method for the ground-state energy of mean-field models up to first order in the inverse particle number. We refine the method for Bosonic systems and obtain bounds for the first-order corrections in the Bosonic and the full case. We apply the theory to the mean-field Ising and the Bose-Hubbard model and relate it to the finite de Finetti problem. Furthermore, we compare the method to the Holstein-Primakoff approximation and propose an extension to a larger class of mean-field models. Finally, we study the time evolution of the fluctuations, propose a conjecture for their dynamics and derive the related Hamiltonian dynamics around the mean-field ground state.

Quantum walks (QWs) are a widely used model system for transport processes on lattices. Initially introduced from a computer science perspective, the field has significantly expanded and is now largely treated from a physics perspective. In fact, “quantum walk” is now widely taken to be synonymous with “discrete time or discrete space quantum dynamics” of a particle with internal degrees of freedom. Experimental implementations of quantum walks with trapped ions showed their strengths in the high fidelity of the results. However, these implementations had two major drawbacks. On the one hand, the protocol for the shift operator allowed for a relatively small number of steps due to its restriction to the Lamb-Dicke regime. On the other hand, the position states, being implemented by coherent states of a harmonic oscillator, were not mutually orthogonal, in contrast to established theoretical models.

In the second part of this thesis, we provide solutions for these drawbacks. On the one hand, we propose a protocol for the shift operator, which is not bound to the Lamb-Dicke regime and therefore allows for a significantly higher number of steps. We provide an error estimation showing that the method allows for up to 100 steps of a QW with state-of-the-art trapped-ion technology. On the other hand, we present a theoretical model for quantum walks with non-orthogonal position states (nQW) and show that these allow for a variety of interesting experiments. In particular, we show that the nQW simulates an (orthogonal) QW with an extended initial state. Moreover, we show that state-of-the-art technology allows for manipulating the spreading rate of the QW, probing the corresponding dispersion relation, and implementing effects from solid-state physics, such as Bloch oscillations.

Keywords: Mean field theory, Many-particle systems, Quantum physics

Zusammenfassung

Vielteilchenquantensysteme bilden ein grundlegendes Forschungsgebiet der Quantenphysik. So bieten diese zum Beispiel eine mikroskopische Beschreibung von makroskopischen Festkörpern, wie zum Beispiel Magneten oder Supraleitern. Ein Ziel ist es, makroskopisch beobachtbare Phänomene, wie Para- oder Ferromagnetismus oder Supraleitung, aus der mikroskopischen Beschreibung herzuleiten. Allerdings ist im Allgemeinen schon die Berechnung der Grundzustandsenergie solcher Systeme in komplexitätstheoretischer Hinsicht nicht möglich, häufig nichteinmal für Quantencomputer. Daher kommen in der Forschung in großem Maße Näherungsverfahren zur Anwendung, wobei eine der häufigsten die Meanfieldtheorie ist. Trotz der extensiven Nutzung dieser existiert allerdings bis dato keine allgemeine Abschätzungsmethode zur Qualität dieser Näherung.

Im ersten Teil dieser Dissertation stellen wir eine algebraische Theorie der Korrekturen erster Ordnung zum Meanfieldlimes von Meanfieldsystemen vor, welche von Raggio und Werner 1989 eingeführt worden sind. Wir nutzen das Konzept sogenannter Fluktuationen, welche zuvor für translationsinvariante Systeme im Sinne eines nichtkommutativen zentralen Grenzwertsatzes verwendet und auch für Meanfieldsysteme in einem rudimentären Maße angewendet worden sind. Wir zeigen, dass diese im Kontext von Meanfieldsystemen eine Algebra mit kanonischen Vertauschungsrelationen erzeugen, welche in einfacher Form die Asymptotik erster Ordnung quantifiziert und als asymptotische Erweiterung über ein Variationsprinzip über Produktzustände hinaus betrachtet werden kann. Wir präsentieren eine detailierte Beschreibung der algebraischen Struktur und identifizieren die jeweiligen Normalmoden. Darauf aufbauend entwickeln wir eine Methode zur Abschätzung der Grundzustandsenergie von Meanfieldmodellen bis zur ersten Ordnung in der inversen Teilchenzahl. Wir verfeinern die Methode zur Anwendung auf Bosonische Systeme und erhalten Abschätzungen der Korrekturen erster Ordnung für den Bosonischen und den allgemeinen Fall. Wir wenden die Theorie auf das Meanfield-Ising und das Bose-Hubbardmodell an und stellen einen Bezug zum endlichen de Finetti-Problem her. Weiterhin vergleichen wir die Methode mit der Holstein-Primakoff-Näherung und schlagen eine Erweiterung auf eine größere Klasse von Meanfieldmodellen vor. Abschließend betrachten wir die Zeitentwicklung von Fluktuatoren, stellen eine Vermutung zu deren Dynamik auf und leiten die entsprechende Hamiltonsche Dynamik um den Grundzustand des Meanfieldsystems her.

Quantenwalks (QWs) sind ein umfassend genutztes Modellsystem zur Beschreibung von Transportprozessen auf Gittern. Aus der ursprünglichen Verwendung im computerwissenschaftlichen Kontext hat sich das Forschungsgebiet stark vergrößert und wird heute weitestgehend im physikalischen Sinne behandelt. In der Tat wird der Begriff "Quantenwalk" heute als Synonym für "Dynamik in diskreter Zeit oder diskretem Raum" eines Teilchens mit internen Freiheitsgraden verstanden. Experimentelle Umsetzungen von QWs mit gefangenen Ionen wiesen ihre Stärke in der hohen Güte der Ergebnisse auf. Allerdings hatten diese Implementationen zwei wesentliche Nachteile. Einerseits erlaubte die verwendete Umsetzung des Shiftoperators aufgrund ihrer Beschränkung auf das Lamb-Dicke Regime nur eine vergleichsweise geringe Anzahl an Schritten. Andererseits waren die Positionszustände, da sie als kohärente Zustände eines harmonischen Oszillators umgesetzt wurden, nicht orthogonal zueinander, im Gegensatz zu den gängigen theoretischen Modellen.

Im zweiten Teil dieser Dissertation präsentieren wir Lösungen zu diesen Problemen. Einerseits schlagen wir eine experimentelle Umsetzung des Shiftoperators vor, welche nicht an das Lamb-Dicke Regime gebunden ist und daher eine signifikant höhere Anzahl an Schritten erlaubt. Mittels einer Fehleranalyse zeigen wir, dass mit dieser Methode bis zu 100 Schritte eines QWs mit der aktuell verfügbaren Technologie bzgl. gefangener Ionen möglich ist. Andererseits stellen wir ein theoretisches Modell für Quantenwalks mit nichtorthogonalen Zuständen (nQW) vor und zeigen, dass diese eine Bandbreite interessanter Experimente ermöglichen. Insbesondere zeigen wir, dass ein nQW einen (orthogonalen) QW simuliert, dessen Anfangszustand verbreitert ist. Darüberhinaus zeigen wir, dass es mittels aktuell verfügbarer Technologie möglich ist, die Ausbreitungsgeschwindigkeit dieses QWs zu manipulieren, die Dispersionsrelation des Walkoperators zu messen, und Phänomene aus der Festkörperphysik, wie zum Beispiel Blochoszillationen, zu erzeugen.

Schlagworte: Meanfieldnäherung, Vielteilchensysteme, Quantenphysik

Preface

This thesis consists of two parts. Part I is on the project of estimating first-order corrections to the mean field limit, while Part II deals with quantum walks with non-orthogonal position states. These two quite different projects are the result of two research lines I pursued during my PhD studies.

Part I of this thesis, the mean field project, was developed out of the attempt to obtain an improved description of the atomic-ensembles experiments by Eugene Polzik [49]. The result is now a theoretical framework that describes the asymptotics towards the mean field limit developed by Raggio, Duffield and Werner [89, 31]. At the time I started my PhD studies in the group of Prof. Dr. Reinhard Werner, this project had already been running. The PhD student Friederike Trimborn and Reinhard Werner worked on estimating the first-order corrections to the ground state energy of mean field models using mean field fluctuations, as a version of a non-commutative central limit theorem [42]. Reinhard and I initially focussed on the time evolution of the mean field fluctuations. We had to leave this project unfinished as we did not succeed in proving the conservation of the fluctuation property for finite times, cf. Sect. 5.3. I decided to finish the ground state estimation project, which was left unfinished by Friederike after she obtained her PhD and left science. Finishing this project proved to be more extensive than expected and provided a variety of interesting results. Most importantly, the concept of scaled fluctuators allowed us to understand the structure of the limiting fluctuation algebra in detail, which furthermore allowed us to refine the ground state estimation to Bosonic particles and to obtain precise bounds for the ground state energy of the related fluctuation Hamiltonian. As will be apparent in the related sections, the results of this thesis allow for quite straightforward extensions and hopefully promising projects. A publication of the results in a scientific journal is currently in preparation.

Part II of this thesis, on quantum walks, grew out of my Diplom[1] studies and was pursued in parallel to the mean field project. For my physics Diplom, I worked on experiments with trapped ions in the group of Prof. Dr. Tobias Schätz. During this time, we successfully demonstrated the experimental implementation of a quantum walk with trapped ions and published the results [101]. However, Tobias and I decided to publish a longer paper as well, which contains a much more detailed description of the experiment and its limitations, as well as a proposal for a better protocol (cf. Section 9) [72]. Furthermore, since the implementation used coherent states of a harmonic oscillator, which are not mutually orthogonal, as the position states of the quantum walk, it was a natural consequence to think of a theoretical model describing quantum walks with non-orthogonal position states. Reinhard and I developed a basic concept

[1]The former german analogue of the master's degree.

that would allow for an interpretation of my numerical observations. Later we decided to work out this project in detail, together with the PhD students Andre Ahlbrecht, Christopher Cedzich and Albert Werner from our group and with Martin Enderlein and Tobias Schätz, supporting us with experimental expertise. The results were published in [72] and [71].

Statement of Contribution

Part I of this thesis shares some content with [111], due to the nature of the project. Part II, on the other hand, contains results that were partly obtained in collaboration. Therefore I will point out my own results and my role in the projects below.

Part I

The project on first-order corrections to the mean field limit was partly carried out in collaboration with Friederike Trimborn and Reinhard Werner. My personal contributions are the following:

Chapter 3

- Def. 3.2.2, the definition of tensor fluctuators.
- Sect. 3.3, derivation of the transformation law between tensor and elementary fluctuators.
- The concept and properties of scaled fluctuators, i.e. Props. 3.4.2 and 3.5.3.
- Lemma 3.5.4 on the expectation value of fluctuators with a filtered sequence of states for finite n.
- Sect. 3.6, on the structure of the fluctuation algebra and the identification of normal modes.

Chapter 4

- Lemma 4.2.1 on the product of the state and gradient.
- Thm. 4.2.2 on the estimation of the ground state energy of a mean field model up to order $1/n$. The basic idea for the inequality was introduced by Trimborn [111], but was true only for the case of the minimizer being in the interior of the state space. The definition of the fluctuation Hamiltonian containing the scaled fluctuator and the identification of its properties was carried out by me.
- Sect. 4.3 on the ground state energy estimation for Bosonic systems.
- Sect. 4.4 on the purification of mean field models, providing a mechanism to map any mean field model to a Bosonic one.

- Sect. 4.5, the application of the ground state energy estimation method to the mean field Ising model. The model itself was studied before, since it is a widely considered toy model. However, the application of our ground state energy estimation method and the analytical expressions for the ground state energy are new.
- Sect. 4.6 on Bosonic systems and the ground state energy estimation for the Bose-Hubbard model. Expressing a Bosonic Hamiltonian in Fock space as a symmetric sequence has been done before [111] as well as the ground state energy estimation for the Bose-Hubbard model in a different way: In [111], Bose symmetry was enforced on the 2-particle level without justifying that this implies Bose symmetry on the n-particle level as well. Effectively, there the full mean field method was applied to an altered model, where, in contrast, in this thesis the Bosonic mean field method is applied to the Bose-Hubbard model.
- Sect. 4.8 on the comparison of our method to the widely used Holstein-Primakoff approximation.
- Sect. 4.9, the proposal of how to extend our method to a larger class of approximately symmetric Hamiltonians.

Chapter 5

- Sect. 5.2, the time evolution of differential forms, which can be considered as a general differential-geometric concept. In our specific context, a rudimentary description was given in [31]. The explicit description in coordinates and the subsequent results were obtained by me.
- Sect. 5.3 on the time evolution of fluctuators.
- Sect. 5.4 on the time evolution of fluctuators for the mean field ground state case.

Part II

The results presented in Chapters 8 and 9 were partly obtained in collaboration with Martin Enderlein, Thomas Huber, Christian Schneider, Hector Schmitz, Jan Glückert and Tobias Schätz. The contributions, which were carried out by myself, are the investigation of the limits of the experimental protocol and the estimation of the feasibility of the photon kicks protocol, with support by Juan Jose Garcia-Ripoll. The related publication, [72], was largely written by me.

The project on quantum walks with non-orthogonal position states, Chapter 10, was carried out in collaboration with Andre Ahlbrecht, Christopher Cedzich, Albert Werner, Martin Enderlein, Michael Keyl, Tobias Schätz, and Reinhard Werner. In this project, I was the lead investigator, in the sense of developing the idea and the project outline, initiating the collaborations and largely writing the publication, [71]. The theoretical model was developed in collaboration with Andre Ahlbrecht, Christopher Cedzich, Albert Werner, Reinhard Werner.

Part II of this thesis contains the publications [72] and [71], which were largely written by me.

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This thesis would not have been possible without the support of numerous people. First of all, I want to thank my supervisor, Reinhard Werner, for giving me the opportunity to obtain my PhD in his group.

Concerning the first year of my PhD studies, I want to thank my former diploma supervisor, Tobias Schätz and friend and co-worker Martin Enderlein for the great collaboration on the extension of the experimental quantum walk project. Out of this, we developed the theory of non-orthogonal quantum walks, together with Andre Ahlbrecht, Christopher Cedzich and Albert Werner. I therefore want to thank them as well for the great collaboration, which included long-running discussions in order to understand the concept and a whole lot of critical and sometimes provocative questions, which greatly sharpened our minds.

The mean-field project was for the most of it difficult and seemingly everlasting. It was in particular in this time good to have friends around, who helped with good comments on the research and a general friendly atmosphere. In particular, I want to express my gratitude to David Gross, Cedric Beny, Ciara Morgan, Jukka Kiukas, Pieter Naaijkens, Courtney Brell and Yoshifumi Nakata. Also, the discussions with Prof. Tobias Osborne on various mean-field related topics were helpful.

The good atmosphere in the office played its part, for which I want to thank Kais Abdelkhalek and Fabian Transchel.

During my PhD studies, I had the opportunity to visit numerous conferences and several research groups to work on different projects and present my own work. First of all, my thank goes again to my supervisor Reinhard Werner for the financial support and giving me the freedom in order to do so. For the kind hospitality, I would like to thank Tobias Schätz, Dietrich Leibfried, Michael Keyl, Benjamin Schlein, Michael Wolf, Matthias Christandl and Norbert Schuch. Special thanks go to Steve Flammia, Steve Bartlett and Andrew Doherty for inviting me to Sydney for a longer research stay and Stephanie Wehner for inviting me to her group in Singapore. Furthermore, a big thank you goes to our secretary, Wiebke Möller, for helping me in organizing the travels and working out the travel forms.

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Contents

Part I.

First-order corrections to the mean-field limit

Notation

$\lvert\psi_\rho\rangle \in \mathcal{H}_p$	Purification of $\rho \in \mathcal{S}(\mathcal{A})$, Lem. 4.4.3.
$\mathcal{A} = \mathcal{B}(\mathcal{H})$	One-particle operator algebra, Sect. 2.2.
$\mathcal{A}_p = \mathcal{B}(\mathcal{H} \otimes \mathcal{K})$	Extended one-particle operator algebra, Def. 4.4.1.
$\mathcal{A}_h \subset \mathcal{A}$	Set of hermitian one-particle operators, Sect. 2.4.
$\mathcal{A}_n \subset \mathcal{A}^{\otimes n}$	The n-particle permutation invariant operator algebra, Sect. 2.2.
A_n	Either element of $\mathcal{A}_n$ or sequence $(A_n)_{n\in\mathbb{N}}$ of elements of $\mathcal{A}_n$, depending on context, Sect. 2.2.
$A_\infty \in \mathcal{C}(\mathcal{S}(\mathcal{A}))$	Limiting function of the approximately symmetric sequence A_n, Eq. (2.13).
$\widetilde{A}$	Elementary fluctuator around ρ, Def. 3.2.1.
$\widetilde{A_k}$	Tensor fluctuator around ρ, Def. 3.2.2.
$\widehat{A}$, $\widehat{A}_k$	Limiting fluctuators around ρ, Def. 3.5.1.
$\widehat{\widehat{A}}$	Scaled fluctuator around ρ, Prop. 3.5.3.
$\mathrm{cov}_\rho(A, B)$	Covariance of $A, B \in \mathcal{A}$ in ρ, Eq. (3.11).
$\mathcal{C}(\mathcal{S}(\mathcal{A}))$	Set of continuous functions on $\mathcal{S}(\mathcal{A})$, Sect. 2.2.
$\mathrm{d}_r f(\rho)$	The r-th derivative of $f \in \mathcal{C}(\mathcal{S}(\mathcal{A}))$ at ρ, Def. 2.4.1 and 2.4.2.
$\mathcal{F}_\rho$	Fluctuation algebra around ρ, Lem. 3.5.2.
$\mathcal{F}_t$	Flow on $\mathcal{S}(\mathcal{A})$ implementing $T_{t,\infty}$, Sect. 2.3.
$\mathrm{Fluct}(A_k)$	Alternative notation for finite-n fluctuators around ρ, Def. 3.2.2.
$\mathrm{Fluct}_\infty(A_k)$	Alternative notation for limiting fluctuators around ρ, Def. 3.5.1.
G_n	Generator of $T_{t,n}$, Sect. 2.3.
G_∞	Generator of $T_{t,\infty}$, Sect. 2.3.
$\mathcal{H}$	One-particle Hilbert space, Sect. 2.2.
$\mathcal{H}_p = \mathcal{H} \otimes \mathcal{K}$	One-particle Hilbert space of the extended mean-field model, Def. 4.4.1.
$\mathcal{H}_n \subset \mathcal{H}^{\otimes n}$	Permutation invariant n-particle Hilbert space, Sect. 2.2.
$\mathcal{H}_\rho$	Hilbert space of the fluctuation algebra around ρ, Def. 3.5.1.
$\widehat{H}(\rho)$	Fluctuation Hamiltonian of a mean-field sequence H_n around a mean-field minimizer $\rho \in \mathcal{S}(\mathcal{A})$, Eq. (4.6).

$\mathrm{id}(A) = A \quad \forall A$	Identity-operator.
$J_t(\rho)$	Jacobian of $\mathcal{F}_t$, Sect. 5.2.
$\Omega \in \mathcal{H}_\rho$	Limiting vector of a sequence ρ_n with root-n fluctuations around ρ, Def. 3.5.1.
$P(A) = \rho(A)\mathbb{1}$	Projector on $\mathcal{A}$, Sect. 3.2.
$\rho \in \mathcal{S}(\mathcal{A})$	A one-particle state. We identify each state ρ (as a functional on $\mathcal{A}$) with its density matrix, which we denote by ρ as well. That is, $\rho(A) = \mathrm{Tr}(\rho \cdot A)$, for $A \in \mathcal{A}$, cf. Sect. 2.2.
$\mathrm{sym}_n(.)$	Symmetrization map $\mathcal{A}^{\otimes k} \mapsto \mathcal{A}_n \; \forall k \leq n$, Eq. (2.3) .
$\mathrm{sym}_\infty(.)$	Map from $\mathcal{A}_n$ onto $\mathcal{C}(\mathcal{S}(\mathcal{A}))$, Eq. (2.12).
$\mathrm{Sym}_n(.)$	Symmetrization map for operators on $\mathcal{A}_n$, Eq. (2.25).
$\mathrm{Sym}_n \, \mathcal{H}^{\otimes n} \subset \mathcal{H}^{\otimes n}$	Bosonic subspace of permutation invariant n-particle Hilbert space, Eq. (2.56).
$\mathcal{S}(\mathcal{A})$	One-particle state space, Sect. 2.2.
$\mathcal{S}_{\mathrm{pure}}(\mathcal{A}) \subset \mathcal{S}(\mathcal{A})$	Subset of pure one-particle states, Sect. 4.3.1.
$\mathcal{S}_\rho(\mathcal{A}) \subset \mathcal{S}(\mathcal{A})$	Subset of one-particle states $U\rho U^*$ for all unitaries U, Sect. 2.4.
$T_{t,n}$	Time-evolution operator on $\mathcal{A}_n$, Sect. 2.3.
$T_{t,\infty}$	mean-field limit of $T_{t,n}$, Sect. 2.3.
$T_\rho \mathcal{S}(\mathcal{A})$	Tangent space at $\rho \in \mathcal{S}(\mathcal{A})$, Sect. 2.4.
$T^*_\rho \mathcal{S}(\mathcal{A})$	Cotangent space at $\rho \in \mathcal{S}(\mathcal{A})$, Sect. 2.4.
$\mathrm{var}_\rho(A) = \mathrm{cov}_\rho(A, A)$	Variance of $A \in \mathcal{A}$ in ρ, Eq. (3.16).
$\mathcal{Y}$	Set of strictly symmetric sequences, Def. 2.2.1.
$\widetilde{\mathcal{Y}}$	Set of approximately symmetric sequences, Def. 2.2.1.

1. Motivation for the project

Many-particle quantum systems are a fundamental research area in quantum physics. For example, they provide the microscopic description of macroscopic solid-state systems, like magnets or superconductors. In order to understand their macroscopically observable properties, like para- or ferromagnetism or superconductivity, beyond phenomenology, it is desirable to derive them from the microscopic description.

Probably the most relevant observable of a many-particle quantum system is the Hamiltonian, modeling the energy. On the one hand, it is the generator of the time evolution of the system; on the other hand, it is the quantity determining macroscopic properties at thermal equilibrium in the thermodynamic limit. More precisely, the partition function, from which most macroscopic observables, such as the free energy or entropy, can be deduced in thermal equilibrium at temperature T, amounts to $Z(T) = \mathrm{Tr}\left(e^{-H/T}\right)$, where H is the Hamiltonian [108].

In the past century, various models (i.e. Hamiltonians) providing a simplified description of realistic solid state systems, were introduced. Prominent examples are the Ising or Heisenberg models, describing atomic lattices, where each atom is equipped with a magnetic moment from a valence electron, for the study of magnetism, or the Hubbard model, describing interacting electrons in an atomic lattice for the study of electric conductivity. Other examples are models describing Bose gases [69], spin glasses [13], atomic nuclei [107], etc..

Often, the low temperature behaviour of such models is of interest. At such temperatures, the lowest eigenvalue of H, modeling the ground-state energy of the system, is dominant in the partition function. Therefore, it is in this case desirable to compute the ground-state energy or even the corresponding ground state. Most straightforwardly, this can be achieved by diagonalizing H. However, it was shown that this task is computationally hard, in some cases even for quantum computers [62, 12, 59, 60, 115] and therefore practically impossible in general for large particle numbers n.

There exist various methods allowing one to approximate the quantities of interest. Prominent examples are density matrix renormalization methods [118, 102], quantum monte carlo methods [38], low-order approximations in path integral formalisms [6] or large-spin expansions in connetion with the Holstein-Primakoff or Schwinger-Boson representation in the sense of spin wave theory [10].

One of the most common approximation methods in many-particle quantum physics is mean-field theory. However, there exist various different concepts of what is called mean-field theory, ranging from the Weiss model over variational methods to saddle point approximations in path integral formalisms. In the following, we will describe a few of these and bring our project into context.

Originally, mean field theory was introduced by P. Weiss in the study of paramagnetic materials, Cf. [55]. His postulated (classical) model consisted of magnetic momenta, which not only interact with an external magnetic field, but also an internal one, which models the collective magnetization of the system and is therefore an average over the bulk of the magnetic moments. Hence, the internal field is a prototype of a mean field, and due to its dependence on the bulk the system energy is computed by solving a nonlinear equation over one particle. E. Ising later refined the model by removing the internal field and introducing an interaction term for neighbouring momenta[1] [55]. By suitable replacement of operator products by single operators multiplied with an expectation value, the Weiss model is obtained as an approximation.

Today, mean field theory is largely understood as a variational ansatz over product states. In particular, this is often used for Bosonic systems, yielding the well-known Gross-Pitaevski equation [47, 86], whereas for Fermionic systems the corresponding variational class is the set of Slater determinants, and the variational principle is commonly known as Hartree-Fock theory [91]. Another instance of a mean field theory for Fermions is the dynamical mean field theory, where e.g. the Hubbard model is mapped to an impurity model and the Green's function is computed there [41]. Moreover, the variational principle over matrix product states[2] of only bond dimension one is exactly a variation over product states and therefore often called mean field theory [114]. On the other hand, a common context for the application of mean field theories are systems at thermal equilibrium at a finite temperature [10]. There, the mean field approximation is often performed on the partition function in the path integral formalism. This type of mean field method is also often called saddle point or stationary phase approximation, referring to the simplification of the action integral [10]. More generally, in terms of Feynman diagrams, mean field theory is often considered as the one-loop approximation. However, it is not clear whether these methods are related to the variational principle over product states.

Despite the extensive usage of mean field theories, general methods to estimate the quality of the approximation do not exist. It is general folklore that the mean field approximation becomes better as the lattice dimension or, more generally, the connectivity among the particles increases. Indeed, for infinite-dimensional lattices, the mean field approximation in the sense of variation over product states becomes exact, and such models are referred to as mean-field models. Infinite lattice dimension can also be understood as long-range interaction, in the sense that all particles interact with each other in the same manner and strength.

The exactness of the mean field approximation as a limit of infinitely many particles on a fully connected lattice (the *mean field limit*) was proved by Duffield, Raggio and Werner for general C^*-algebras [89, 88, 90, 29, 30, 31, 28, 117]. Their theory, in par-

[1] This, as well is the Weiss model, is a classical one, where each magnetic moment can be in one of two states. The quantum Ising model consists of spin-$\frac{1}{2}$ quantum particles. In this thesis, we focus on the quantum models.

[2] It was shown, that the density matrix renormalization group is a variational principle over matrix product states [80, 32].

ticular the papers [89, 31, 29], are the basis of the project presented in this thesis. It was shown that the mean field limit can be described by a classical system, namely a commutative C*-algebra over the one-particle state space. That is, the quantumness of the system is not observable in this limit.

In Part I of this thesis, we derive an algebraic description of the $1/n$-asymptotics towards the infinite-particle limit $n \to \infty$. We use a concept called *fluctuations*, which has been previously used in translationally invariant systems [42] in the sense of a non-commutative central limit theorem and has been applied to mean-field models in a basic manner before [52]. We show that in the context of mean-field models, where we call them *mean-field fluctuations*, they give rise to an algebra of canonical commutation relations (CCR), which is closely connected to the phase space of the mean-field limit and conveniently describes the asymptotic behaviour. The purpose of the fluctuation algebra is to quantify expectation values of observables in sequences of n-particle states that are beyond product states. That is, the fluctuation algebra allows for the extension of the variational class of states beyond the product states in an asymptotic sense. Furthermore, we will use the concept of mean-field fluctuations to estimate the ground-state energy of mean-field models up to order $1/n$ and apply it to various examples.

In the following, we outline the rest of Part I of this thesis. In Chapter 2, we review the basics of the mean field theory derived in [89, 31, 29]. We restrict the general C*-algebraic theory to finite-dimensional matrix algebras, which are the systems of interest in this thesis. In particular, we outline the proof of the convergence towards the mean-field limit for observables. Furthermore, we describe the mean-field limit for the time evolution as well, in particular for Hamiltonian dynamics, and describe the differential-geometric structure of the limiting algebra. Finally, we provide an overview of the properties of permutation invariant operators and states.

In Chapter 3, we introduce the concept of mean-field fluctuations and derive the structure of the limiting fluctuation algebra. In particular, we introduce three classes of fluctuators. These are *elementary* and *tensor fluctuators*, which are related by a transformation rule, as well as *scaled fluctuators*, which are essentially one order higher in $1/\sqrt{n}$. We show the relation between fluctuators and elements of the phase space of the mean-field limiting algebra. Then we introduce sequences of states with *root-n fluctuations*, which allow for taking the infinite-particle limit of the fluctuators, being described by a CCR algebra. We provide a range of results concerning the structure of the algebra. In particular, we identify the normal modes and scaled fluctuators.

In Chapter 4, we use the fluctuation method to estimate the ground-state energy[3] up to order $1/n$ for a class of mean-field Hamiltonians. We derive a general inequality yielding an upper bound for the ground-state energy, where the related $1/n$-coefficient is given by the ground-state energy of a quadratic Hamiltonian in the corresponding

[3]More precisely, throughout this thesis we will consider the energy per particle. That is, while the total energy of a mean-field system is proportional to the particle number n, we will consider the energy divided by n, such that the leading order of what we call the *ground-state energy* is constant and the next order proportional to $1/n$.

fluctuation algebra. We restrict the theory to Bosonic systems and derive bounds on the ground-state energy of the fluctuation Hamiltonian. Using purification methods, we extend these bounds to the general mean-field case, where no particle statistics are assumed. We apply the ground-state energy estimation to the mean-field Ising model as well as the Bose-Hubbard model, and for the latter, we show that the fluctuation Hamiltonian is exactly the well-known Bogoliubov Hamiltonian [85]. Furthermore, we show the relation between the mean-field ground-state problem and the finite de Finetti problem [23] in the sense that an inner bound can be obtained by minimizing over a set of fluctuation Hamiltonians. Finally, we describe the relation of the fluctuation method to the Holstein-Primakoff approximation and show that the latter is a special case of the former. We finish the chapter by proposing an extension of the fluctuation method to a larger class of mean-field Hamiltonians.

In Chapter 5, we consider the time evolution of mean-field fluctuations. First, we outline the time evolution of differential forms, i.e. elements of the phase space of the mean-field limiting algebra. Then we cite a result on fluctuation dynamics for a slightly different class of Hamiltonians [52] and provide arguments that suggest the same theorem may be true for the class of Hamiltonians considered in this thesis. Since we were not able to derive a rigorous proof, we leave it as a conjecture. Finally, we refine the conjecture to the evolution of fluctuations around a ground state in the mean-field limit and show that in this case the time evolution of fluctuators is generated exactly by the fluctuation Hamiltonian that gives rise to the $1/n$-corrections to the mean-field ground-state energy.

In Chapter 6, we summarize Part I of this thesis and provide an overview over open questions and possible extensions of the mean-field and fluctuation project.

2. Generalized mean-field theory

2.1. Overview

In this chapter, we describe the generalized mean field theory, which was developed in [89]. This theory is the basis for the subject of this thesis, the first-order corrections to the corresponding mean-field limit. After initially proving the emergence of the Gibbs-variational principle for mean-field systems [89], a series of papers was published, describing dynamical properties and related topics [88, 31, 29, 30, 28, 90].

Throughout this thesis, we will consider systems consisting of finite-dimensional quantum particles with Hamiltonian dynamics. Hence, we will restrict the description of mean field theory to such systems, although it applies to general C*-algebras.

In Section 2.2, we define mean-field models as n-particle systems and derive the algebraic structure of the limit of infinitely many particles, i.e. the structure of the mean-field limiting algebra, which is represented by a commutative algebra of continuous functions on the one-particle state space $\mathcal{S}(\mathcal{A})$ [89]. In Section 2.3, we derive the mean-field limit of Hamiltonian dynamics, which is implemented by a nonlinear Hamiltonian flow on $\mathcal{S}(\mathcal{A})$ [31]. In Section 2.4, we derive the symplectic structure of the manifold $\mathcal{S}(\mathcal{A})$, emphasizing the classicality of the mean-field limit. We will introduce the tangent and cotangent spaces and define derivatives of functions. These will be of particular importance for the derivation of the $1/n$-corrections to the mean-field ground-state energy. Finally, in Section 2.5, we present a few aspects and results concerning permutation invariant operators and states from a different perspective.

2.2. Mean-field models

In this section, we define mean-field models and describe their mathematical structure. mean-field models are many-particle systems, for which the mean field approximation becomes exact in the limit of infinitely many particles. Their defining property is invariance of the observables under permutations of the particles[1].

Let $\mathcal{A} = \mathcal{B}(\mathcal{H})$ with $\dim \mathcal{H} = d$ denote the C*-algebra of bounded operators acting on a Hilbert space, describing the set of observables of a one-particle system. The norm of an element $A \in \mathcal{A}$ is given by the operator norm

$$\|A\| = \sup_{|\psi\rangle \in \mathcal{H}} \frac{\|A|\psi\rangle\|}{\||\psi\rangle\|}. \tag{2.1}$$

[1]However, this does not mean that we restrict to Bosonic or Fermionic particle statistics, cf. Sect. 2.5.

We denote states of the one-particle system $\mathcal{A}$ by $\rho \in \mathcal{S}(\mathcal{A})$, where $\mathcal{S}(\mathcal{A}) \subset \mathcal{B}^*(\mathcal{H})$ denotes the set of positive operators with unit trace[2]. Throughout this thesis, we will exchangably treat states as density matrices and as functionals on $\mathcal{A}$, in the operator-algebraic sense, without distinguishing the notation. That is, the expectation value of an observable $A \in \mathcal{A}$ in $\rho \in \mathcal{S}(\mathcal{A})$ will be denoted by

$$\rho(A) \equiv \mathrm{Tr}(\rho \cdot A), \tag{2.2}$$

where Tr(.) denotes the trace of the related matrix. Many-particle systems are modeled by the composition of one-particle systems. That is, a system of n copies of a particle $\mathcal{A}$ is modeled by the algebra $\mathcal{A}^{\otimes n} = \mathcal{A} \otimes \mathcal{A} \otimes ... \otimes \mathcal{A}$, the n-fold tensor product of $\mathcal{A}$.

The n-particle algebra of a mean-field model, $\mathcal{A}_n \subset \mathcal{A}^{\otimes n}$, is spanned by operators that are invariant under permutations of the tensor factors. The permutation invariance allows us to embed k-particle operators into n-particle systems, for $n \geq k$, by the symmetrization map $\mathrm{sym}_n : \mathcal{A}^{\otimes k} \to \mathcal{A}_n$, which is defined by

$$\mathrm{sym}_n(A_k) = \frac{1}{n!} \sum_{\pi \in \mathcal{S}_n} \pi \left(A_k \otimes \mathbb{1}^{\otimes n} \right) \quad \forall A_k \in \mathcal{A}^{\otimes k}, \tag{2.3}$$

where $\pi(X_1 \otimes ... \otimes X_n) = X_{\pi(1)} \otimes ... \otimes X_{\pi(n)}$ is an automorphism permuting the tensor factors, i.e. a representation of the element $\pi \in \mathcal{S}_n$ of the n-particle permutation group, and the sum goes over all such permutations. In Section 2.5, we will provide a few more details on representations of the permutation group, which are not required here. The symmetrization map thus maps k-particle operators into permutation invariant n-particle operators for all $n \geq k$. In fact, it is sufficient to consider only permutation invariant k-particle operators A_k, due to the chaining property $\mathrm{sym}_n = \mathrm{sym}_n \circ \mathrm{sym}_k$ $\forall k \leq n$. Therefore, throughout this thesis, for every $A_n = \mathrm{sym}_n A_k$, the operator A_k is assumed to be invariant under permutations, if not stated differently. Using this map, we construct two types of sequences.

Definition 2.2.1. *A sequence of operators, $A = (A_n)_n$, with $A_n \in \mathcal{A}_n$, is called*

- *strictly symmetric, if $\exists A_k \in \mathcal{A}_k$ such that*

$$A_n = \mathrm{sym}_n A_k \quad \forall n \geq k \tag{2.4}$$

- *approximately symmetric, if $\forall \epsilon > 0 \, \exists N_\epsilon \in \mathbb{N}$ such that*

$$\| A_n - \mathrm{sym}_n A_m \| < \epsilon \quad \forall n \geq m \geq N_\epsilon. \tag{2.5}$$

We denote the set of strictly or approximately symmetric sequences by $\mathcal{Y}$ or $\widetilde{\mathcal{Y}}$, respectively.

[2]For finite dimensional Hilbert spaces, $\mathcal{B}(\mathcal{H})$ and $\mathcal{B}^*(\mathcal{H})$ are isomorphic. However, we will keep the formal distinction, which will be convenient in Section 2.4.

The symmetrization map sym_n does not increase the norm, i.e.

$$\|\mathrm{sym}_n A_k\| = \frac{1}{n!}\left\|\sum_\pi \pi\left(A_k \otimes \mathbb{1}^{\otimes n}\right)\right\| \le \frac{1}{n!}\sum_\pi \left\|\pi\left(A_k \otimes \mathbb{1}^{\otimes n}\right)\right\| = \|A_k\|. \tag{2.6}$$

Therefore, we identify the symmetric sequences with *intensive* observables, i.e. those for which measurement outcomes do not depend on the particle number. The product of two strictly symmetric sequences is approximately symmetric:

$$\mathrm{sym}_n A_k \cdot \mathrm{sym}_n B_l = \sum_{r=0}^{\min(k,l)} c_n(k,l,r)\,\mathrm{sym}_n\Big(\left(A_k \otimes \mathbb{1}^{\otimes(l-r)}\right)\cdot\left(\mathbb{1}^{\otimes(k-r)} \otimes B_l\right)\Big), \tag{2.7}$$

where

$$c_n(k,l,r) = \frac{k!l!(n-k)!(n-l)!}{r!n!(k-r)!(l-r)!(n-k-l+r)!}, \tag{2.8}$$

which asymptotically amounts to

$$\lim_{n\to\infty} n^r c_n(k,l,r) = r!\binom{k}{r}\binom{l}{r}. \tag{2.9}$$

Since, to leading order in $1/n$, the product of two strictly symmetric sequences amounts to

$$\mathrm{sym}_n A_k\,\mathrm{sym}_n B_l = \mathrm{sym}_n(A_k \otimes B_l) + O\left(\frac{1}{n}\right), \tag{2.10}$$

the symmetrization map can be considered as an asymptotic homomorphism. Furthermore, the commutator between two symmetric sequences vanishes in the limit, i.e.

$$\|[\mathrm{sym}_n A_k, \mathrm{sym}_n B_l]\| = O\left(\frac{1}{n}\right). \tag{2.11}$$

That is, in the limit of infinitely many particles, the operators are abelian and hence by the Gelfand-Naimark theorem [18] elements of the C*-algebra of continuous functions on a compact Hausdorff space. In the following, we make this limit construction and the structure of the algebra precise.

For each $A_n \in \mathcal{A}_n$, define the function $\mathrm{sym}_\infty A_n \in \mathcal{C}(\mathcal{S}(\mathcal{A}))$ by

$$\mathrm{sym}_\infty A_n(\rho) := \rho^{\otimes n}(A_n) \quad \forall \rho \in \mathcal{S}(\mathcal{A}). \tag{2.12}$$

Furthermore, for a sequence A_n, define the limiting function

$$\begin{aligned} A_\infty(\rho) &:= \lim_{n\to\infty} \mathrm{sym}_\infty A_n(\rho) \\ &= \lim_{n\to\infty} \rho^{\otimes n}(A_n), \end{aligned} \tag{2.13}$$

which clearly exists for all strictly symmetric sequences. Indeed, for $A_n = \mathrm{sym}_n A_k$, we have $\rho^{\otimes n}(\mathrm{sym}_n A_k) = \rho^{\otimes k}(A_k)$ for all $n \ge k$. That is, strictly symmetric sequences are in one-to-one correspondence to polynomials of finite degree on $\mathcal{S}(\mathcal{A})$. Due to (2.10), the map (2.13) is a homomorphism.

On $\widetilde{\mathcal{Y}}$, we define the seminorm

$$\|A\| = \lim_{n\to\infty} \|A_n\| . \tag{2.14}$$

Under this seminorm, $\widetilde{\mathcal{Y}}$ is an abelian algebra of sequences with element-wise addition and multiplication, i.e. $(A+B)_n = A_n+B_n$ and $(A\cdot B)_n = A_n\cdot B_n$, and $\mathcal{Y}$ is a dense subset. Hence, the map (2.13) exists on the whole $\widetilde{\mathcal{Y}}$, and the limiting functions $A_\infty \in \mathcal{C}(\mathcal{S}(\mathcal{A}))$ can be considered as representatives of equivalence classes w.r.t. the equivalence relation

$$A \sim B :\Leftrightarrow \lim_{n\to\infty} \|A_n - B_n\| = 0 \quad \forall A, B \in \widetilde{\mathcal{Y}}. \tag{2.15}$$

Due to (2.7) and (2.6), the map (2.13) is an isometric *-homomorphism from $\widetilde{\mathcal{Y}}$ to the abelian C*-algebra $\mathcal{C}(\mathcal{S}(\mathcal{A}))$, with commutator-sequences $([A_n, B_n])_n$ being in its kernel. $\mathcal{C}(\mathcal{S}(\mathcal{A}))$ is also called the Hausdorff completion of $\mathcal{Y}$. We summarize the construction by citing the following proposition.

Proposition 2.2.2 ([89, 31])**.**

1. *For every $A \in \widetilde{\mathcal{Y}}$, the seminorm $\|A\| = \lim_{n\to\infty} \|A_n\|$ exists. $\widetilde{\mathcal{Y}}$ is the completion of $\mathcal{Y}$ in this seminorm, in the sense that $\forall \epsilon > 0\, \exists A^\epsilon \in \mathcal{Y}$ such that $\|A - A^\epsilon\| < \epsilon$. Moreover, $\widetilde{\mathcal{Y}}$ is closed within the set of all sequences $n \mapsto A_n \in \mathcal{A}_n$ in this seminorm.*

2. *$\widetilde{\mathcal{Y}}$ is an algebra of sequences with element-wise addition $(A + B)_n = A_n + B_n$ and multiplication $(AB)_n = A_n B_n$. Furthermore, it is commutative under the seminorm, i.e.*
$$\|AB - BA\| = \lim_{n\to\infty} \|A_n B_n - B_n A_n\| = 0. \tag{2.16}$$

3. *For all $A \in \widetilde{\mathcal{Y}}$, $A_\infty(\rho) = \lim_{n\to\infty} \mathrm{sym}_\infty A_n(\rho)$ exists uniformly for $\rho \in \mathcal{S}(\mathcal{A})$.*

4. *The map*
$$\widetilde{\mathcal{Y}} \to \mathcal{C}\big(\mathcal{S}(\mathcal{A})\big) : A \to A_\infty \tag{2.17}$$
is an isometric *-homomorphism onto $\mathcal{C}\big(\mathcal{S}(\mathcal{A})\big)$.

As an example, we consider the mean-field Ising model in a transverse magnetic field. The corresponding Hamiltonian can be written as

$$nH_n = B \sum_{i=1}^{n} \sigma_z^{(i)} + \frac{J}{n-1} \sum_{i\neq j=1}^{n} \sigma_x^{(i)} \sigma_x^{(j)}, \tag{2.18}$$

where $\sigma_\alpha^{(i)} = \mathbb{1}^{\otimes(i-1)} \otimes \sigma_\alpha \otimes \mathbb{1}^{\otimes(n-i)}$ for $\alpha \in \{x, y, z\}$. In this model, all particles interact with each other, since the second sum goes over all i and j independently. The factor $1/(n-1)$ can be seen as a normalization to compare systems with different particle numbers n. Indeed, each particle has $n-1$ interaction partners. Note that we defined the Hamiltonian as nH_n, where H_n itself is called *Hamiltonian density* or *energy per particle*. Clearly, the Hamiltonian density can be written as $H_n = \mathrm{sym}_n H_2$ with

$$H_2 = \frac{1}{2}(\sigma_z \otimes \mathbb{1} + \mathbb{1} \otimes \sigma_z) + J\sigma_x \otimes \sigma_x \tag{2.19}$$

and is therefore a strictly symmetric sequence. The mean-field limiting function, H_∞, is evaluated as $H_\infty(\rho) = \rho^{\otimes 2}(H_2)$. The ground-state estimation of this model is performed in Section 4.5. Sometimes in the literature a similar model is considered, where the factor on the interaction term amounts to $1/n$ instead of $1/(n-1)$. Since $1/n = (1 - 1/n)/(n-1)$, this model amounts to an approximately symmetric sequence, given by $H_n = \mathrm{sym}_n H_2 - (1/n)\,\mathrm{sym}_n(J\sigma_x \otimes \sigma_x)$.

2.3. The mean-field limit of Hamiltonian dynamics

In this section, we consider the time evolution of mean-field models and see, under which conditions a mean-field limit of the time-evolved system exists and what its structure is. The mean-field limit of the time evolution was worked out in [31] for general C*-algebras and later, in [29], made precise for Hamiltonian dynamics on finite dimensional C*-algebras.

We start by stating the general conditions for the existence of the mean-field limit of the time evolution and then give the details for finite dimensional Hamiltonian dynamics.

On $\mathcal{A}_n$, the n-particle mean-field system, consider the quantum dynamical semigroup $T_{t,n}\colon \mathcal{A}_n \to \mathcal{A}_n$ with $t \geq 0$, describing the time evolution of the system. Given a Hamiltonian nH_n, the time evolution can be written as

$$T_{t,n}A_n = e^{itnH_n} A_n e^{-itnH_n}, \tag{2.20}$$

with unitary operators $e^{\pm itnH_n} \in \mathcal{A}_n$. The generator of the time evolution is given by $G_n A_n = i[nH_n, A_n]$.

In the following, we consider $\left(T_{t,n} = e^{tG_n}\right)_{t\geq 0}$ as a strongly continuous one-parameter semigroup of identity-preserving contractions on $\mathcal{A}_n$. Furthermore, for every fixed t, consider $T_{t,n}$ as a sequence in n. Clearly, if the mean-field limit of the time-evolved system is supposed to exist, the following condition is needed: If A_n is an approximately symmetric sequence, then $T_{t,n}A_n$ has to be approximately symmetric as well[3]. The following lemma ensures that the limit of the sequence $T_{t,n}$ (for t fixed) is well defined.

Lemma 2.3.1 ([31])**.** *Let T_n: $\mathcal{A}_n \to \mathcal{A}_n$ be a uniformly bounded sequence of operators, which intertwine the symmetrization map* sym_n*. Then the following conditions are equivalent:*

1. *For all $A_n \in \widetilde{\mathcal{Y}}: T_n A_n \in \widetilde{\mathcal{Y}}$.*
2. *For all $A_n \in \widetilde{\mathcal{Y}}$:* $\lim_{m\to\infty} \lim_{n\to\infty} \left\|\left(\mathrm{sym}_n T_m - T_n \,\mathrm{sym}_n\right) A_m\right\| = 0$.
3. *For all $A_n \in \widetilde{\mathcal{Y}}$:* $\lim_{n\geq m\to\infty} \left\|\left(\mathrm{sym}_n T_m - T_n \,\mathrm{sym}_n\right) A_m\right\| = 0$.

If these conditions are satisfied, then T_∞: $A_\infty \mapsto \left(T_. A_.\right)_\infty$ is well-defined and the sequence T_n will be called approximate symmetry preserving.

[3]In the following we will denote sequences $(A_n)_n$ just by A_n, whenever the contetxt is clear, or by $A_.$.

Hence, for fixed t, if $T_{t,\cdot}$ is approximate symmetry preserving, then the operator $T_{t,\infty}\colon A_\infty \mapsto \big(T_{t,\cdot}A_\cdot\big)_\infty = T_{t,\infty}A_\infty$ is well defined. However, it is desireable to find conditions, under which the $T_{t,\infty}$, with t being a parameter, define a strongly continuous semigroup of contractions with generator G_∞. Indeed, this is the case if the resolvents of G_n,

$$R_n(s) = (s - G_n)^{-1} = \int_0^\infty \mathrm{d}t\, e^{-st} T_{t,n}, \tag{2.21}$$

for $s \in \mathbb{C}$ with $\mathrm{Re}(s) > 0$ are approximate symmetry preserving and map $\widetilde{\mathcal{Y}}$ onto a dense subset of $\widetilde{\mathcal{Y}}$. Then the limiting operators $R_\infty(s)$ define the generator G_∞. The following theorem ensures the existence of the mean-field limit of a dynamical semigroup.

Theorem 2.3.2 ([31])**.** *For each $n \in \mathbb{N}$, let $\big(T_{t,n} = e^{tG_n}\big)_{t\geq 0}$ be a strongly continuous one-parameter semigroup of contractions on $\mathcal{A}_n$ with generator G_n, and let $s \in \mathbb{C}$,* $\mathrm{Re}(s) > 0$. *Then the following are equivalent:*

1. *$T_{t,n}$ is approximate symmetry preserving, and strongly continuous in the sense that for all $A_n \in \widetilde{\mathcal{Y}}$,*
$$\lim_{\substack{t\to 0\\ n\to\infty}} \|T_{t,n}A_n - A_n\| = 0. \tag{2.22}$$
2. *For each t, $T_{t,n}$ is approximate symmetry preserving, and the set of sequences A_n with $A_n \in \mathrm{Dom}(G_n)$ and $\|G_nA_n\|$ uniformly bounded, is dense in $\widetilde{\mathcal{Y}}$.*
3. *$R_n(s)$ is approximate symmetry preserving, and $\big\{R_n(s)A_n \,|\, A_n \in \widetilde{\mathcal{Y}}\big\}$ is dense in $\widetilde{\mathcal{Y}}$.*
4. *There is a dense linear subspace $\mathcal{D} \subset \widetilde{\mathcal{Y}}$ such that $\big\{(G_n - s)A_n \,|\, A_n \in \mathcal{D}\big\}$ is dense in $\widetilde{\mathcal{Y}}$.*
5. *G_∞ is well-defined, closed, and generates a semigroup of contractions on $\mathcal{C}\big(\mathcal{S}(\mathcal{A})\big)$.*

If these conditions are satisfied, then $\mathfrak{Dom}(G_n) = \big\{R_n(s)A_n \,|\, A_n \in \widetilde{\mathcal{Y}}\big\}$ and $T_{t,\infty} = e^{tG_\infty}$ is the mean-field limit of $T_{t,n}$.

Here, $\mathrm{Dom}(G_n)$ is the domain of the linear operator G_n on the n-particle system $\mathcal{A}_n$ and $\mathfrak{Dom}(G_n)$ is the domain of the sequence $(G_n)_n$, defined by

$$\mathfrak{Dom}(G_n) = \big\{(A_n)_n \in \widetilde{\mathcal{Y}} \,\big|\, A_n \in \mathrm{Dom}(G_n)\ \forall n, \text{ and } (G_nA_n)_n \in \widetilde{\mathcal{Y}}\big\}. \tag{2.23}$$

Therefore, the mean-field limit of $T_{t,n}$ is a strongly continuous semigroup of *–homomorphisms $T_{t,\infty}$ on $\mathcal{C}(\mathcal{S}(\mathcal{A}))$. In [97] it was shown that the semigroup is implemented by a continuous flow on $\mathcal{S}(\mathcal{A})$. More precisely, if X is a compact space, then there is a correspondence between strongly continuous contraction semigroups $(T_t)_{t\geq 0}$ on $\mathcal{C}(X)$, that are *-homomorphisms and preserve the identity function, linear operators Z on $\mathcal{C}(X)$, that generate contraction semigroups on $\mathcal{C}(X)$ and are *-derivations, and continuous flows $(F_t)_{t\geq 0}$ on X. The correspondence is given by

$$T_t f = e^{tZ} f = f \circ F_t \quad \forall f \in \mathcal{C}(X). \tag{2.24}$$

In [31], two classes of time evolutions that have a mean-field limit, were presented. The related generators were called bounded polynomial and approximately polynomial.

Consider G_k as a bounded operator on $\mathcal{A}_k$ for some $k \in \mathbb{N}$. In analogy to the symmetrization map (2.3), we define a symmetrization map to bounded operators on $\mathcal{A}_n$, for $n \geq k$, by

$$\mathrm{Sym}_n G_k = \frac{1}{n!} \sum_\pi \pi \left(G_k \otimes \mathrm{id}^{\otimes n-k} \right) \circ \pi^{-1}, \tag{2.25}$$

where $\mathrm{id}(A) = A$ for all $A \in \mathcal{A}$. A bounded polynomial generator is a sequence $(G_n)_n$ of bounded operators G_n on $\mathcal{A}_n$, such that

$$G_n = \frac{n}{k} \mathrm{Sym}_n G_k, \tag{2.26}$$

where G_k is the generator of a norm-continuous semigroup of completely positive unital maps on $\mathcal{A}_k$. The notion "bounded" stems from the fact that $\|G_n\| \leq \frac{n}{k} \|G_k\|$ for $n \geq k$. In this thesis, we will consider almost entirely such generators defined by Hamiltonians. Let $H_n = \mathrm{sym}_n H_k$ be a strictly symmetric sequence of hermitian operators. Then

$$G_n(A_n) = in[H_n, A_n] \tag{2.27}$$

is a bounded polynomial generator of degree k. We call nH_n the Hamiltonian and H_n the Hamiltonian density, describing the energy per particle. Clearly, $G_n A_n$ is an approximately symmetric sequence for any approximately symmetric A_n, due to the product rule (2.7). Hence, G_n preserves approximate symmetry and has a limit G_∞. Consider $T_{t,n}$ as the dynamical semigroup generated by G_n. In [31] it was shown that for any $A_n \in \widetilde{\mathcal{Y}}$, $T_{t,n} A_n$ is approximately symmetric with a uniform convergence on the intervall $0 \leq t \leq \tau$ with $\tau = (2^{g-1} \|G_g\|)^{-1}$. By iteration, it follows that $T_{t,n}$ is approximate symmetry preserving for all $t \geq 0$. Moreover, it has a mean-field limit $T_{t,\infty}$, which is generated by G_∞ [31].

In the next section, we make G_∞ and $T_{t,\infty}$ explicit using concepts of differential geometry.

2.4. The symplectic structure of the mean-field algebra

In this section, we investigate the structure of the state space $\mathcal{S}(\mathcal{A})$ of the one-particle algebra $\mathcal{A} = \mathcal{B}(\mathcal{H})$ with $\dim \mathcal{H} = d$. We consider $\mathcal{S}(\mathcal{A})$ as a manifold. At each point $\rho \in \mathcal{S}(\mathcal{A})$ we define a tangent space

$$T_\rho \mathcal{S}(\mathcal{A}) = \left\{ \phi \in \mathcal{A}^* \middle| \phi = \phi^*, \, \phi(\mathbb{1}) = 0 \right\}, \tag{2.28}$$

where $\mathcal{A}^*$ denotes the dual of $\mathcal{A}$. The dual of $T_\rho \mathcal{S}(\mathcal{A})$ it is the cotangent space $T^*_\rho \mathcal{S}(\mathcal{A})$. It is defined by the bilinear form

$$\langle ., . \rangle : T_\rho \mathcal{S}(\mathcal{A}) \times T^*_\rho \mathcal{S}(\mathcal{A}) \to \mathbb{R}, \tag{2.29}$$

which is the restriction of the bilinear form $\mathcal{A}^* \times \mathcal{A} \mapsto \mathbb{C}$ onto the elements of $T_\rho \mathcal{S}(\mathcal{A})$. Hence, the cotangent space amounts to

$$T^*_\rho \mathcal{S}(\mathcal{A}) = \mathcal{A}_h \big/ \mathbb{R}\mathbb{1}, \tag{2.30}$$

where $\mathcal{A}_h$ denotes the set of hermitian elements in $\mathcal{A}$. The following definition of a derivative holds for general C*-algebras.

Definition 2.4.1 ([29]). *A function $f \in \mathcal{C}(\mathcal{S}(\mathcal{A}))$ is called differentiable, if*

1. *for all $\rho \in \mathcal{S}(\mathcal{A})$, there exists a hermitian element $\mathrm{d}f(\rho) \in \mathcal{A}$, such that for all $\sigma \in \mathcal{S}(\mathcal{A})$*
$$\langle \sigma - \rho, \mathrm{d}f(\rho)\rangle = \lim_{\mu \searrow 0} \frac{1}{\mu}\Big(f\big((1-\mu)\rho + \mu\sigma\big) - f(\rho)\Big) \tag{2.31}$$
exists as a weak- continuous affine functional on $\sigma \in \mathcal{S}(\mathcal{A})$, and*
2. *the maps $\rho \mapsto \langle \sigma - \rho, \mathrm{d}f(\rho)\rangle$ are weak-* continuous, uniformly for $\sigma \in \mathcal{S}(\mathcal{A})$.*

By this definition, the gradient $\mathrm{d}f(\rho)$ is an equivalence class in $\mathcal{A}$ not just in $\mathcal{A}^{**}$. Hence, it suffices to require continuity in the weak-* topology instead of the weak topology. We fix a representative for the gradient by the convention $\rho\big(\mathrm{d}f(\rho)\big) = 0$. With this, $\mathrm{d}f(\rho)$ is a unique element of $\mathcal{A}$ and item (2) of the above definition can be rewritten, saying that the map $\rho \mapsto \mathrm{d}f(\rho)$ is weak–*–to–norm continuous. Moreover, an expectation value of $\mathrm{d}f(\rho)$ can then be written as

$$\sigma\big(\mathrm{d}f(\rho)\big) = \frac{\mathrm{d}}{\mathrm{d}\mu} f\big((1-\mu)\rho + \mu\sigma\big)\Big|_{\mu=0}. \tag{2.32}$$

Throughout this thesis, we will also use a notion of differentials for one-particle operators, instead of functions. That is, we define

$$\mathrm{d}X(\rho) := X - \rho(X)\mathbb{1} \quad \forall X \in \mathcal{A}, \tag{2.33}$$

which is just a short form for considering the sequence $X_n = \mathrm{sym}_n X$ and then the related differential $\mathrm{d}X_\infty(\rho)$.

We define higher derivatives $\mathrm{d}_r f(\rho)$ of f in the same fashion. That is for example, for the second derivative of f at a point ρ, we demand the existence of

$$\frac{\mathrm{d}^2}{\mathrm{d}\mu \mathrm{d}\nu} f\big((1-\mu-\nu)\rho + \mu\sigma + \nu\omega\big)\Big|_{\substack{\mu=0\\ \nu=0}} = \frac{\mathrm{d}}{\mathrm{d}\mu}\Big\langle \omega - \rho, \mathrm{d}f\big(\rho + \mu(\sigma-\rho)\big)\Big\rangle\Big|_{\mu=0} \quad \forall \sigma, \omega \in \mathcal{S}(\mathcal{A}). \tag{2.34}$$

Hence, we require now that the map $\sigma \mapsto \langle \sigma - \rho, \mathrm{d}f(\rho)\rangle$ is not just weak-* continuous, but even differentiable at ρ. A general way to define such a derivative, is to consider a function of the type $\Phi\colon \mathcal{S}(\mathcal{A}) \to \mathcal{B}$, where $\mathcal{B}$ is a general C*-algebra. We fix a $\sigma_0 \in \mathcal{S}(\mathcal{B})$ and consider the restricted function

$$\sigma_0(\Phi(.))\colon \mathcal{S}(\mathcal{A}) \to \mathbb{R}, \tag{2.35}$$

for which we apply the above definition of the first derivative. Hence, the differential of Φ at $\rho \in \mathcal{S}(\mathcal{A})$ into the direction $\sigma \in \mathcal{S}(\mathcal{A})$, evaluated with $\sigma_0 \in \mathcal{S}(\mathcal{B})$ amounts to

$$\sigma \otimes \sigma_0\big(\mathrm{d}\Phi(\rho)\big) = \frac{\mathrm{d}}{\mathrm{d}\mu}\sigma_0\Big(\Phi\big((1-\mu)\rho + \mu\sigma\big)\Big)\Big|_{\mu=0}. \tag{2.36}$$

Thus, $\mathrm{d}\Phi(\rho) \in \mathcal{A}\otimes\mathcal{B}$. Therefore, we obtain the r-th derivative of the function $f\colon \mathcal{S}(\mathcal{A}) \to \mathbb{R}$ by iterating this construction, and see that it is given by the element $\mathrm{d}_r f(\rho) \in \mathcal{A}^{\otimes r}$. In fact, an expectation value of it can be computed by

$$\sigma_1 \otimes \sigma_2 \otimes \ldots \otimes \sigma_r\big(\mathrm{d}_r f(\rho)\big) = \frac{\mathrm{d}^r}{\mathrm{d}\mu_1 \ldots \mathrm{d}\mu_r} f\big((1-\mu_1 \ldots - \mu_r)\rho + \mu_1\sigma_1 \ldots + \mu_r\sigma_r\big)\big|_{\mu_1,\ldots,\mu_r=0}. \tag{2.37}$$

Since the value is independent of the order of derivatives, the operator $\mathrm{d}_r f(\rho)$ is permutation invariant, hence an element in $\mathcal{A}_r \subset \mathcal{A}^{\otimes r}$. It is therefore sufficient for the definition, to evaluate it with product states. Moreover, as the derivative of a real-valued function, it must be hermitian.

Definition 2.4.2. *A function $f \in \mathcal{C}(\mathcal{S}(\mathcal{A}))$ is called r times differentiable, if*

1. *for all $\rho \in \mathcal{S}(\mathcal{A})$, there exists a hermitian element $\mathrm{d}_r f(\rho) \in \mathcal{A}_r$, such that for all $\sigma \in \mathcal{S}(\mathcal{A})$*
$$\big\langle(\sigma-\rho)^{\otimes r}, \mathrm{d}_r f(\rho)\big\rangle = \frac{\mathrm{d}^r}{\mathrm{d}\mu^r} f\big((1-\mu)\rho + \mu\sigma\big)\big|_{\mu=0} \tag{2.38}$$
exists as a weak- continuous affine functional on $\sigma \in \mathcal{S}(\mathcal{A})$, and*

2. *the maps $\rho \mapsto \langle(\sigma-\rho)^{\otimes r}, \mathrm{d}_r f(\rho)\rangle$ are weak-* continuous, uniformly for $\sigma \in \mathcal{S}(\mathcal{A})$.*

Again, we consider $\mathrm{d}_r f(\rho) \in \mathcal{A}_r$ uniquely as the representative of the equivalence class by choosing the convention

$$\rho \otimes \sigma_{r-1}\big(\mathrm{d}_r f(\rho)\big) = 0 \quad \forall \sigma_{r-1} \in \mathcal{S}(\mathcal{A}_{r-1}) \tag{2.39}$$

and update the definition to saying that $\rho \mapsto \mathrm{d}_r f(\rho)$ is weak-*–to–norm continuous.

The definition of derivatives allows us now to introduce the Taylor expansion of polynomial functions [111]. Consider the strictly symmetric sequence $H_n = \mathrm{sym}_n H_k$. Then $H_\infty(\rho) = \rho^{\otimes k}(H_k)$ is a polynomial of degree k. We can perform a Taylor expansion on such a function in the following way

$$\begin{aligned} H_\infty(\sigma) &= \sum_{r=0}^{k} \frac{1}{r!}\frac{\mathrm{d}^r}{\mathrm{d}t^r} H_\infty\big((1-t)\rho + t\sigma\big)\big|_{t=0} \\ &= \sum_{r=0}^{k} \frac{1}{r!}\sigma^{\otimes r}\big(\mathrm{d}_r H_\infty(\rho)\big) \\ &= \sum_{r=0}^{k} \frac{1}{r!}\sigma^{\otimes n}\big(\mathrm{sym}_n\, \mathrm{d}_r H_\infty(\rho)\big) \quad \forall n \geq k. \end{aligned} \tag{2.40}$$

Since this expansion holds for all $\sigma, \rho \in \mathcal{S}(\mathcal{A})$, we can identify the n-particle operators as

$$H_n = \sum_{r=0}^{k} \frac{1}{r!} \operatorname{sym}_n\big(\mathrm{d}_r H_\infty(\rho)\big) \quad \forall \rho \in \mathcal{S}(\mathcal{A}). \tag{2.41}$$

With the Taylor expansion, we can make the limit G_∞ of a bounded polynomial generator $G_n(.) = in[H_n, .]$, with $H_n = \operatorname{sym}_n H_k$, explicit. Consider a strictly symmetric sequence $A_n = \operatorname{sym}_n A_l$. Then the sequence $in[H_n, A_n]$ is approximately symmetric and, using the product rule (2.7) and Taylor expansion (2.41), can be written as

$$\begin{aligned} G_n A_n &= in[H_n, A_n] \\ &= \sum_{r=1}^{k} \sum_{s=1}^{l} \frac{1}{r!} \frac{1}{s!} in\big[\operatorname{sym}_n \mathrm{d}_r H_\infty(\sigma), \operatorname{sym}_n \mathrm{d}_s A_\infty(\sigma)\big] \\ &= \sum_{r=1}^{k} \sum_{s=1}^{l} \frac{k}{r!} \frac{l}{s!} i \operatorname{sym}_n\big[\mathrm{d}_r H_\infty(\sigma) \otimes \mathbb{1}^{\otimes l-1}, \mathbb{1}^{\otimes k-1} \otimes \mathrm{d}_s A_\infty(\sigma)\big] + O\left(\frac{1}{n}\right) \end{aligned} \tag{2.42}$$

for all $\sigma \in \mathcal{S}(\mathcal{A})$. Hence, the limiting function $G_\infty A_\infty$ is a polynomial of the leading order terms of (2.42) and $G_\infty A_\infty(\rho)$ is given by their evaluation with product states $\rho^{\otimes n}$, for n large enough. But since $\rho \otimes \sigma_{x-1}(\mathrm{d}_x f(\rho)) = 0$, we can perform the above expansion (2.42) at ρ, the point at which the function is evaluated, such that all leading order terms vanish, except the one with the first derivatives. That is,

$$G_\infty A_\infty(\rho) = \rho\big(i[\mathrm{d}H_\infty(\rho), \mathrm{d}A_\infty(\rho)]\big). \tag{2.43}$$

This result also holds for approximately symmetric A_n with a differentiable limiting function and a broader class of Hamiltonian densities H_n [29]. On the level of functions on $\mathcal{S}(\mathcal{A})$, we define the following bracket for differentiable $f, g \in \mathcal{C}(\mathcal{S}(\mathcal{A}))$,

$$\{f, g\}(\rho) = \eta\big(\mathrm{d}f(\rho), \mathrm{d}g(\rho)\big) = \rho\big(i[\mathrm{d}f(\rho), \mathrm{d}g(\rho)]\big), \tag{2.44}$$

where $\eta\colon \mathcal{A}_h \times \mathcal{A}_h \to \mathbb{R}$ defines an antisymmetric bilinear form on $T^*_\rho \mathcal{S}(\mathcal{A})$. Hence, $G_\infty(.) = \{H_\infty, .\}$ is a derivation, generating the mean-field time evolution $T_{t,\infty}$. The corresponding flow $\mathcal{F}_t \rho = \rho_t$ is obtained by the cyclicity of the trace, that is

$$\begin{aligned} \{H_\infty, g\}(\rho) &= \rho\big(i[\mathrm{d}H_\infty(\rho), \mathrm{d}g(\rho)]\big) \\ &= \operatorname{Tr}\big(\rho \cdot i[\mathrm{d}H_\infty(\rho), \mathrm{d}g(\rho)]\big) \\ &= \operatorname{Tr}\big(-i[\mathrm{d}H_\infty(\rho), \rho] \cdot \mathrm{d}g(\rho)\big). \end{aligned} \tag{2.45}$$

Hence, the flow is defined by the following differential equation, known as the Hartree equation [29]

$$\frac{\mathrm{d}}{\mathrm{d}t} \mathcal{F}_t \rho = \dot{\rho}_t = -i[\mathrm{d}H_\infty(\rho_t), \rho_t]. \tag{2.46}$$

Therefore, we obtain the identification $T_{t,\infty} A_\infty(\rho) = A_\infty(\rho_t)$.

It is important to note, that $\{., .\}$ is not a proper Poisson bracket, since it is degenerate. In particular, if $[\rho, \mathrm{d}f(\rho)] = 0$, then $\{f, .\}(\rho) \equiv 0$. However, there exists a foilation of

$\mathcal{S}(\mathcal{A})$, such that the restriction of the bracket to the leaves is indeed non-degenerate and closed, meaning that the leaves are proper symplectic submanifolds [29]. In the following, we outline the construction of the foilation by considering at each point ρ a subspace $\mathcal{N}_\rho^\perp \subset T_\rho\mathcal{S}(\mathcal{A})$, on which the bracket is non-degenerate. Then we will show that the $\mathcal{N}_\rho^\perp$ are tangent spaces of submanifolds of $\mathcal{S}(\mathcal{A})$.

Define

$$\mathcal{N}_\rho = \left\{A \in T_\rho^*\mathcal{S}(\mathcal{A}) \,\middle|\, \eta(B,A) = 0\, \forall B \in \mathcal{A}_h\right\}, \tag{2.47}$$

which is non-empty. The set of tangent vectors $\phi_H \in T_\rho\mathcal{S}(\mathcal{A})$ with $\langle\phi_H, A\rangle = \eta(H,A)$ for some $H \in \mathcal{A}$ is a proper subspace of the tangent space. This subspace is just the orthogonal complement $\mathcal{N}_\rho^\perp$ of $\mathcal{N}_\rho$, since for every $\phi_H \in \mathcal{N}_\rho^\perp$, $\eta(H,A) = 0$ for all $A \in \mathcal{N}_\rho$. By taking the quotient, η is non-degenerate on

$$T_\rho^*\mathcal{S}(\mathcal{A})\big/\mathcal{N}_\rho. \tag{2.48}$$

Its dimension amounts to $\dim T_\rho^*\mathcal{S}(\mathcal{A})\big/\mathcal{N}_\rho = \dim T_\rho^*\mathcal{S}(\mathcal{A}) - \dim\mathcal{N}_\rho = \dim\mathcal{N}_\rho^\perp$ and must be even, due to the non-degeneracy of η on $\mathcal{N}_\rho^\perp$. It remains to be shown that the $\mathcal{N}_\rho^\perp$ are tangent spaces of a submanifold $\mathcal{S}_\rho$ through ρ. Since by construction all Hamiltonian vector fields point along $\mathcal{N}_\rho^\perp$, the submanifold $\mathcal{S}_\rho$ is identified by computing the flows for all those vector fields starting from ρ. For any Hamiltonian function h, the related flow $\mathcal{F}_t$ is generated by the related Hartree equation (2.46). By considering $H_t \equiv \mathrm{d}h(\rho_t)$ as a time-dependent Hamiltonian, one can write down a differential equation for unitary operators

$$\frac{\mathrm{d}}{\mathrm{d}t}U_t = iU_tH_t, \qquad U_0 = \mathbb{1}. \tag{2.49}$$

and obtain

$$(\mathcal{F}_t\rho)(A) = \rho(U_tAU_t^*) \quad \forall A \in \mathcal{A}, \tag{2.50}$$

where U_t is by construction an element of the identity component G_0 of the unitary group in $\mathcal{A}$.

Hence, the symplectic submanifold $\mathcal{S}_\rho$, which is a leaf of the foilation of $\mathcal{S}(\mathcal{A})$, is spanned by the points $U\rho U^*$, with $U \in G_0$, or can just be considered as the homogeneous space $G_0\big/G_\rho$, where G_ρ is the subgroup of G_0 consisting of elements that fulfill $U\rho U^* = \rho$. If we consider $\mathcal{A}$ as the matrix algebra of $d\times d$ matrices, i.e. $\mathcal{A} = \mathcal{M}_d$, then the structure of $\mathcal{S}_\rho$ depends on the eigenvalues p_i of ρ and their multiplicities d_i. The unitaries that leave ρ invariant, are elements of $\bigoplus_i \mathcal{M}_{d_i}$, corresponding to the multiplicities d_i. Since the tangent spaces of G_0 and G_ρ are given by the hermitian elements of $\mathcal{M}_d$ and $\bigoplus_i \mathcal{M}_{d_i}$, respectively, we get $\dim G_0 = d^2$ and $\dim G_\rho = \sum_i d_i^2$. Therefore, the dimension of the leaf $\mathcal{S}_\rho$ is $d^2 - \sum_i d_i^2$, which is even [29].

In Chapter 4, we will extensively use the symplectic submanifold of pure states, $\mathcal{S}_{\text{pure}}(\mathcal{A}) \subset \mathcal{S}(\mathcal{A})$.

2.5. Properties of permutation invariant operators and states

In this section, we present a few aspects and results concerning permutation invariant operators and states from a different perspective. The purpose is to give the reader an intuition about the structure of these. The first part of this section essentially follows [43].

We start with an introduction of the permutation group $\mathcal{S}_n$. Consider the set of n natural numbers $\{1, 2, ..., n\}$. An element $\pi \in \mathcal{S}_n$ is a rule of rearranging the order of the numbers and its action can be written as

$$\pi\{1, 2, ..., n\} = \{\pi(1), \pi(2), ..., \pi(n)\}. \tag{2.51}$$

The simplest instance is the group S_2, which consists of two elements, namely the identity $\mathrm{id}\{1, 2\} = \{1, 2\}$ and the flip $F\{1, 2\} = \{2, 1\}$. Consider the Hilbert space $\mathcal{H}$ with $\dim \mathcal{H} = d$ and the n-fold tensor product $\mathcal{H}^{\otimes n}$. A representation of $\mathcal{S}_n$ on $\mathcal{H}^{\otimes n}$ is given by the unitary operators U_π for $\pi \in \mathcal{S}_n$ with the rule

$$U_\pi |\psi_1\rangle \otimes |\psi_2\rangle \otimes ... \otimes |\psi_n\rangle = \left|\psi_{\pi(1)}\right\rangle \otimes \left|\psi_{\pi(2)}\right\rangle \otimes ... \otimes \left|\psi_{\pi(n)}\right\rangle. \tag{2.52}$$

This representation is reducible and there exists a block decomposition into irreducibles with corresponding multiplicities as

$$U_\pi = \bigoplus_Y U_{\pi,\mathcal{H}_Y} \otimes \mathbb{1}_{\mathcal{K}_Y}, \tag{2.53}$$

where the direct sum runs over all Young diagrams of n boxes arranged in d rows, $\mathcal{H}_Y$ is the related irreducible representation space and $\mathcal{K}_Y$ quantifies the related multiplicity. This decomposition into irreducible representations implies a decomposition of permutation invariant operators. Let $A_n \in \mathcal{B}(\mathcal{H}^{\otimes n})$ be permutation invariant, i.e. $\pi(A_n) = U_\pi^* A_n U_\pi = A_n$ for all $\pi \in \mathcal{S}_n$. Then

$$A_n = \bigoplus_Y \mathbb{1}_{\mathcal{H}_Y} \otimes A_{n,\mathcal{K}_Y}, \tag{2.54}$$

with a collection of matrices $A_{n,\mathcal{K}_Y}$. This decomposition holds for permutation invariant states $\rho_n \in \mathcal{B}(\mathcal{H}^{\otimes n})$ as well[4]. Moreover, we can write

$$\rho_n = \bigoplus_Y w_{\rho_n,Y} \cdot \frac{\mathbb{1}_{\mathcal{H}_Y}}{\dim \mathcal{H}_Y} \otimes \rho_{n,\mathcal{K}_Y}, \tag{2.55}$$

where each tensor factor is a density matrix itself and the non-negative weights $w_{\rho_n,Y} \in \mathbb{R}$ fulfill $\sum_Y w_{\rho_n,Y} = 1$. Of special importance is the trivial representation of U_π, namely the Young diagram Y_1, for which $U_{\pi,\mathcal{H}_{Y_1}} = 1$ for all $\pi \in \mathcal{S}_n$. The related multiplicity space $\mathcal{K}_{Y_1}$ is exactly the Bosonic subspace of $\mathcal{H}^{\otimes n}$, i.e.

$$\mathcal{K}_{Y_1} = \mathrm{Sym}_n\, \mathcal{H}^{\otimes n} = \mathrm{span}\left\{|\psi\rangle \in \mathcal{H}^{\otimes n},\, U_\pi |\psi\rangle = |\psi\rangle\ \forall \pi \in \mathcal{S}_n\right\}. \tag{2.56}$$

A permutation invariant state ρ_n is called Bosonic, iff $w_{\rho_n,Y_1} = 1$, i.e. has full weight on the Bosonic subspace.

[4] This is the only section in this thesis, where we do not keep the formal distinction between $\mathcal{B}(\mathcal{H}^{\otimes n})$ and its dual $\mathcal{B}^*(\mathcal{H}^{\otimes n})$.

The Schur-Weyl duality is a relation between the permutation group $\mathcal{S}_n$ and the general linear group $GL(d)$ of linear maps on a d-dimensional Hilbert space. In our context, the duality relation concerns the reducible representation of $GL(d)$ on $\mathcal{H}^{\otimes n}$, given by $GL(d) \ni A \mapsto A^{\otimes n} \in \mathcal{B}(\mathcal{H}^{\otimes n})$. Clearly $A^{\otimes n}$ is permutation invariant for every $A \in GL(d)$. Therefore, the representation on $\mathcal{H}^{\otimes n}$ is decomposed into irreducibles via

$$A^{\otimes n} = \bigoplus_{Y} \mathbb{1}_{\mathcal{H}_Y} \otimes \left(A^{\otimes n}\right)_{\mathcal{K}_Y}, \tag{2.57}$$

where $\left(A^{\otimes n}\right)_{\mathcal{K}_Y} \in \mathcal{B}(\mathcal{K}_Y)$. It follows that every permutation invariant operator B_n must be decomposable as a linear combination of operators $A^{\otimes n}$. Indeed, consider the set of operators $\mathcal{B}(\mathcal{H})$ as a Hilbert space itself, with the Hilbert-Schmidt inner product $\langle A, B\rangle = \mathrm{Tr}(A^* B)$. Then the polarization identity, Lem. 2.5.1, holds.

Lemma 2.5.1 (Polarization [43]). *Consider a finite dimensional Hilbert space $\mathcal{K}$. The symmetric subspace $\mathrm{Sym}_n \mathcal{K}^{\otimes n}$ of $\mathcal{K}^{\otimes n}$ is spanned by the product vectors $|\psi\rangle^{\otimes n}$ for $|\psi\rangle \in \mathcal{K}$ and the following identity holds*

$$\mathrm{sym}_n(|\psi_1\rangle \otimes |\psi_2\rangle \otimes \ldots \otimes |\psi_n\rangle) = \frac{1}{n! 2^{(n-1)}} \sum_{\epsilon_j = \pm 1} \left(\prod_{j=2}^{n}\right) \left(|\psi_1\rangle + \epsilon_2 |\psi_2\rangle + \ldots + \epsilon_n |\psi_n\rangle\right)^{\otimes n}, \tag{2.58}$$

where $\mathrm{sym}_n(.)$ denotes the normalized sum over all permutations of the tensor factors.

Moreover, Lem. 2.5.1 says that the Bosonic vectors of $\mathcal{H}^{\otimes n}$ are spanned by product vectors $|\psi\rangle^{\otimes n}$.

It is important to note, that linear combinations are not convex combinations. The latter is related to a result of Størmer, extending the original de Finetti theorem [25] to infinite tensor products of C* algebras [109].

Proposition 2.5.2 (Størmer [109]). *Consider the C^*-algebra $\mathcal{A}^\infty$ of infinite copies of the C^*-algebra $\mathcal{A}$. For every permutation invariant state Φ on $\mathcal{A}^\infty$, there exists a unique probability measure μ on $\mathcal{S}(\mathcal{A})$, such that*

$$\Phi = \int_{\mathcal{S}(\mathcal{A})} \mu(\mathrm{d}\phi) \phi^\infty, \tag{2.59}$$

where ϕ^∞ denotes the infinite product state of $\phi \in \mathcal{S}(\mathcal{A})$, in the sense that every reduced state $\Phi^{(n)}$ on $\mathcal{A}^n$ has the form

$$\Phi^n = \int_{\mathcal{S}(\mathcal{A})} \mu(\mathrm{d}\phi) \phi^n. \tag{2.60}$$

The set of states Φ is a Choquet simplex, with the extremal points being identified with the point measures on $\mathcal{S}(\mathcal{A})$.

In other words, Prop. 2.5.2 tells that a for an (infinite) sequence of permutation invariant states $\rho_n \in \mathcal{S}(\mathcal{A}_n)$, with the reduced-state property $\rho_m = \mathrm{Tr}_{n-m}(\rho_n)$ for all $n \geq m$, there exists a unique probability measure μ on $\mathcal{S}(\mathcal{A})$, such that

$$\rho_n = \int_{\mathcal{S}(\mathcal{A})} \mu(\mathrm{d}\rho) \rho^{\otimes n} \quad \forall n. \tag{2.61}$$

Moreover, if the states ρ_n are Bosonic, then the probability measure μ is supported only by the pure states of $\mathcal{A}$. Furthermore, Prop. 2.5.2 can be derived as a corollary of the mean-field theorem 2.2.2 [31].

Another important property of de Finetti states is that as convex combinations of product states they are exactly the set of separable permutation invariant states on $\mathcal{A}_k$ for any $k \in \mathbb{N}$. Hence, a permutation invariant state ρ_k is entangled, iff it is not of de-Finetti type. In this sense, the mean-field limit H_∞ of a strictly symmetric Hamiltonian density $H_n = \mathrm{sym}_n H_k$ corresponds to the evaluation of H_k with separable states of $\mathcal{S}(\mathcal{A}_k)$. In the spirit of finding the ground-state energy of H_n, we wish to minimize H_k over reduced states $\rho_n^{(k)} = \mathrm{Tr}_{n-k}\,\rho_n$ of permutation invariant states $\rho_n \in \mathcal{S}(\mathcal{A}_n)$. States $\rho_n^{(k)}$ of this kind are called n-exchangable. By definition, the set of n-exchangable states contains the de Finetti states as a subset. Furthermore, it contains the set of m-exchangable states for every $m \leq n$. The finite de Finetti theorem, Thm. 2.5.3, gives a bound on the distance to the de Finetti states

Theorem 2.5.3 (Finite de Finetti [23])**.** *Consider a permutation invariant n-particle state $\rho_n \in \mathcal{S}(\mathcal{A}_n)$. There exists a probability measure μ on $\mathcal{S}(\mathcal{A})$, such that for every $k \leq n$,*

$$\left\| \rho_n^{(k)} - \int_{\mathcal{S}(\mathcal{A})} \mu(\mathrm{d}\rho)\rho^{\otimes k} \right\|_1 \leq \frac{2kd^2}{n}, \tag{2.62}$$

where $d = \dim \mathcal{H}$ for $\mathcal{A} = \mathcal{B}(\mathcal{H})$ and $\|.\|_1$ denotes the trace norm [78].

In the spirit of finding the ground-state energy of $H_n = \mathrm{sym}_n H_k$, we would need to minimize H_k over the set of n-exchangable states. However, even for large n, there does not exist a convenient parametrization of such states on $\mathcal{A}_k$. The approach used in this thesis, namely the mean-field fluctuations, allows for a convenient asymptotic parametrization, as we will show in the subsequent chapters. A different interesting concept of extending the variational class beyond product states is given by the set of *almost product states* [64, 63]. It is not obvious, how this concept relates to mean-field fluctuations, in particular, since the set of almost product states is defined in the Schur-Weyl picture, in the sense of Eq. (2.54) and does not use a reference state $\rho \in \mathcal{S}(\mathcal{A})$, in contrast to the definition of mean-field fluctuations, cf. Chapt. 3. However, there exists a method for implementing the concept of mean-field fluctuations into the Schur-Weyl decomposition in the spirit of Eq. (2.54) [56]. It would be interesting to see a general connection between these concepts.

3. The algebra of mean-field fluctuations

3.1. Overview

In this section, we introduce the concept of mean-field fluctuations, in the spirit of a non-commutative central limit theorem. Fluctuations and non-commutative central limits have been introduced before and studied by Verbeure et al. in the context of translation invariant systems on quasi-local algebras [42, 113]. For mean-field models, fluctuations were used for the first time by Hepp and Lieb in their seminal paper [52] and basics have been worked out by Trimborn [111]. Furthermore, closely related concepts are used by Schlein et al. for mean-field systems consisting of infinite-dimensional Bosons [100] and, somewhat less related, by Guta et al. in terms of quantum local asymptotic normality in the spirit of quantum state estimation [57].

While the mean-field limit of a strictly symmetric Hamiltonian corresponds to the evaluation of the finite-n system with product states, cf. Eq. (2.13), the essential idea of mean-field fluctuations is to implicitly define sequences of states ρ_n, which are beyond that. More precisely, we define a class of strictly symmetric operators, called *fluctuators*, which diverge in norm by orders of $\sqrt{n}$ and have vanishing expectation in states related to a reference $\rho \in \mathcal{S}(\mathcal{A})$. The sequences ρ_n of interest are defined by leading to converging expectation values of products of these fluctuators and are said to have *root-n fluctuations around (the reference) ρ*. These sequences need not be of de-Finetti type, i.e. separable. Indeed, for finite n, they can be anything, since the definition concerns only the asymptotic behaviour. The latter is then described in terms of the *limiting fluctuation algebra*.

In this chapter, we introduce the definitions of fluctuators, sequences with root-n fluctuations and the limiting fluctuation algebra. We study their properties and algebraic structure in detail. Furthermore, we identify the relation between mean-field fluctuations around a reference $\rho \in \mathcal{S}(\mathcal{A})$ and elements of the phase space $T^*_\rho\mathcal{S}(\mathcal{A})$ in the mean-field limit. Moreover, we identify the normal modes of the corresponding limiting fluctuation algebra $\mathcal{F}_\rho$.

The rest of this chapter is ordered as follows. In Section 3.2, we provide the definition of fluctuators as operators on the n-particle systems. In particular, we provide two definitions, namely of *elementary* and *tensor fluctuators*, both of which will be relevant in the subsequent chapters. In Section 3.3, we derive a recursive transformation rule between elementary and tensor fluctuators for finite n and in the limit $n \to \infty$. We will use the transformation throughout Chapter 4. In Section 3.4, we compute the limits of expectation values of fluctuators around $\rho \in \mathcal{S}(\mathcal{A})$ with the product state sequence $\rho^{\otimes n}$. The given propositions will be the basis for most proofs in the subsequent sections. In Section 3.5, we introduce the definition of the limiting fluctuation algebra $\mathcal{F}_\rho$ along with the definition of root-n fluctuations for sequences ρ_n. We show that the algebra satisfies canonical commutation relations (CCR) and study its structure in detail. Moreover, we introduce the concept of scaled fluctuators, which will be relevant in the subsequent chapters as well. Finally, in Section 3.6, we fix a basis, in which the reference state $\rho \in \mathcal{S}(\mathcal{A})$ is diagonal, and identify the normal modes of the fluctuation algebra, the central elements and the scaled fluctuators.

3.2. Definition of fluctuators

In this section, we define the concept of fluctuators, following previous results on non-commutative central limits [52, 42, 111]. Let $\mathcal{A} = \mathcal{B}(\mathcal{H})$ be the algebra of bounded operators acting on the d-dimensional Hilbert space $\mathcal{H}$, describing one particle. Consider a state $\rho \in \mathcal{S}(\mathcal{A})$ and define the projector

$$\mathcal{P}A = \rho(A)\mathbb{1} \quad \forall A \in \mathcal{A}. \tag{3.1}$$

In the following, we omit writing the identity, when its presence is clear from the context.

Definition 3.2.1. *Let $A \in \mathcal{A}$ and $\mathcal{P}A = \rho(A)\mathbb{1}$. Then*

$$\widetilde{A} = \sqrt{n}\,\mathrm{sym}_n\big((\mathrm{id} - \mathcal{P})A\big) \tag{3.2}$$

*is called an **(elementary) fluctuator** around ρ.*

Moreover, the following generalized definition will be useful in Chapter 4.

Definition 3.2.2. *Let $A_k \in \mathcal{A}_k$, then*

$$\widetilde{A_k} = n^{\frac{k}{2}}\,\mathrm{sym}_n\big((\mathrm{id} - \mathcal{P})^{\otimes k} A_k\big) \tag{3.3}$$

*is called a **tensor fluctuator** around ρ.*

Notation–wise, if the expression under the tilde is too wide, we will alternatively use $\mathrm{Fluct}(A_k) := \widetilde{A_k}$. Moreover, the notation carries implicitly the dependence on n and ρ, where the latter is treated as a fixed parameter. An important class of fluctuators is defined by derivatives $\mathrm{d}_k f(\rho)$ of differentiable functions $f \in \mathcal{C}(\mathcal{S}(\mathcal{A}))$. By Def. 2.4.2 they fulfill the property

$$(\mathrm{id} - \mathcal{P})^{\otimes k}(\mathrm{d}_k f(\rho)) = \mathrm{d}_k f(\rho), \tag{3.4}$$

hence the object $\widetilde{\mathrm{d}_k f}(\rho) = n^{\frac{k}{2}}\,\mathrm{sym}_n\big(\mathrm{d}_k f(\rho)\big)$ is a tensor fluctuator around ρ. In the following lemma, we show that every fluctuator corresponds to the derivative of some function.

Lemma 3.2.3. *For every k-particle operator A_k, there exists a k-times differentiable function $f \in \mathcal{C}(\mathcal{S}(\mathcal{A}))$ such that*

$$\widetilde{\mathrm{d}_k f}(\rho) = \widetilde{A_k} \tag{3.5}$$

with any reference state $\rho \in \mathcal{S}(\mathcal{A})$.

Proof. Given A_k, define $B_k = \frac{1}{k!}A_k$ and the sequence $B_n = \mathrm{sym}_n B_k$. Then the desired function is B_∞. Using the Taylor expansion (2.41), we can write

$$\begin{aligned}(\mathrm{id}-\mathcal{P})^{\otimes k}A_k &= (\mathrm{id}-\mathcal{P})^{\otimes k}k!B_k \\ &= (\mathrm{id}-\mathcal{P})^{\otimes k}k!\sum_{r=0}^{k}\frac{1}{r!}\,\mathrm{sym}_k\big(\mathrm{d}_r B_\infty(\rho)\big) \\ &= (\mathrm{id}-\mathcal{P})^{\otimes k}\mathrm{d}_k B_\infty(\rho)\end{aligned} \tag{3.6}$$

and therefore the statement of the lemma. The third line in the computation follows from $(\mathrm{id}-\mathcal{P})\mathbb{1} = 0$, that is $(\mathrm{id}-\mathcal{P})^{\otimes k}\,\mathrm{sym}_k(C_l) = 0$ for every $C_l \in \mathcal{A}^{\otimes l}$ with $l < k$. □

3.3. Transforming tensor fluctuators into elementary fluctuators and vice versa

In the limit $n \to \infty$, the elementary fluctuators are the convenient ones to work with. But higher derivatives of functions, $\mathrm{d}_k f(\rho)$, are tensor fluctuators. Therefore, we give in the following a rule for decomposing tensor fluctuators into elementary ones and vice versa. Consider a general permutation invariant operator $A_k \in \mathcal{A}_k$. Viewed as a vector in the Hilbert-Schmidt space $\mathcal{A}^{\otimes k}$, and using the polarization identity, Lem. 2.5.1, there exist finitely many $A_i \in \mathcal{A}$, such that

$$A_k = \sum_i A_i^{\otimes k}. \tag{3.7}$$

By linearity, we can therefore decompose tensor fluctuators to $\widetilde{A_k} = \sum_i \widetilde{A_i^{\otimes k}}$. In the following, we derive a recursive formula for decomposing fluctuators of the type $\widetilde{A^{\otimes k}}$ into polynomials of elementary fluctuators. We start by computing the product of two such tensor fluctuators. To simplify notation, we write

$$\underline{A} = (\mathrm{id}-\mathcal{P})A = A - \rho(A)\mathbb{1}. \tag{3.8}$$

Using (2.7), the product between $\widetilde{A^{\otimes k}}$ and $\widetilde{B^{\otimes l}}$ amounts to

$$\widetilde{A^{\otimes k}}\cdot\widetilde{B^{\otimes l}} = n^{\frac{k+l}{2}}\sum_{r=0}^{\min(k,l)} c_n(k,l,r)\,\mathrm{sym}_n\Big(\underline{A}^{\otimes k-r}\otimes\underline{B}^{\otimes l-r}\otimes(\underline{A}\cdot\underline{B})^{\otimes r}\Big). \tag{3.9}$$

The overlap terms can be reduced in the following way

$$\begin{aligned}\underline{A}\cdot\underline{B} &= \big(A-\rho(A)\mathbb{1}\big)\big(B-\rho(B)\mathbb{1}\big) \\ &= AB \pm \rho(AB) - \rho(A)B \pm \rho(A)\rho(B) - A\rho(B) \pm \rho(A)\rho(B) + \rho(A)\rho(B) \\ &= \mathrm{cov}_\rho(A,B)\mathbb{1} + \big(\underline{AB} - \rho(A)\underline{B} - \rho(B)\underline{A}\big),\end{aligned} \tag{3.10}$$

where we introduced the covariance

$$\mathrm{cov}_\rho(A,B) = \rho(AB) - \rho(A)\rho(B) = \rho\big((A-\rho(A)\mathbb{1})(B-\rho(B)\mathbb{1})\big) \tag{3.11}$$

and $\underline{AB} = AB - \rho(AB)\mathbb{1}$. Hence,

$$(\underline{A} \cdot \underline{B})^{\otimes r} = \sum_{s=0}^{r} \binom{r}{s} \operatorname{cov}_\rho(A,B)^{r-s} \cdot \operatorname{sym}_r \left(\mathbb{1}^{\otimes r-s} \otimes \left(\underline{AB} - \rho(A)\underline{B} - \rho(B)\underline{A} \right)^{\otimes s} \right). \tag{3.12}$$

Therefore, Eq. (3.9) can be further decomposed into

$$\begin{aligned}
\widetilde{A^{\otimes k}} \cdot \widetilde{B^{\otimes l}} &= \sum_{r=0}^{\min(k,l)} \sum_{s=0}^{r} \binom{r}{s} n^{\frac{k+l}{2}} c_n(k,l,r) \operatorname{cov}_\rho(A,B)^{r-s} \\
&\quad \times \operatorname{sym}_n\Big(\underline{A}^{\otimes k-r} \otimes \underline{B}^{\otimes l-r} \otimes \left(\underline{AB} - \rho(A)\underline{B} - \rho(B)\underline{A} \right)^{\otimes s} \Big) \\
&\sim \sum_{r=0}^{\min(k,l)} \sum_{s=0}^{r} r! \binom{k}{r}\binom{l}{r}\binom{r}{s} \operatorname{cov}_\rho(A,B)^{r-s} n^{\frac{k+l-2r}{2}} \\
&\quad \times \operatorname{sym}_n\Big(\underline{A}^{\otimes k-r} \otimes \underline{B}^{\otimes l-r} \otimes \left(\underline{AB} - \rho(A)\underline{B} - \rho(B)\underline{A} \right)^{\otimes s} \Big) \\
&\sim \sum_{r=0}^{\min(k,l)} \sum_{s=0}^{r} r! \binom{k}{r}\binom{l}{r}\binom{r}{s} \operatorname{cov}_\rho(A,B)^{r-s} n^{-\frac{s}{2}} \\
&\quad \times \operatorname{Fluct}\Big(\underline{A}^{\otimes k-r} \otimes \underline{B}^{\otimes l-r} \otimes \left(\underline{AB} - \rho(A)\underline{B} - \rho(B)\underline{A} \right)^{\otimes s} \Big) \\
&\sim \sum_{r=0}^{\min(k,l)} r! \binom{k}{r}\binom{l}{r} \operatorname{cov}_\rho(A,B)^{r} \cdot \operatorname{Fluct}\Big(A^{\otimes k-r} \otimes B^{\otimes l-r} \Big) + O\left(\frac{1}{\sqrt{n}} \right),
\end{aligned} \tag{3.13}$$

where in the second line we considered only the asymptotic behaviour of $c_n(k,l,r)$, given by Eq. (2.9). In the third line, we wrote the symmetrized operators as fluctuators, using the notation $\operatorname{Fluct}(A_k) = \widetilde{A_k}$, and in the fourth line we considered only the leading-order fluctuators. Hence, the $O\left(\frac{1}{\sqrt{n}}\right)$ is meant as *in expectation*, in a sense specified in Section 3.5, and not in operator norm, in which fluctuators diverge. A special case is the following

$$\begin{aligned}
\operatorname{Fluct}\left(A^{\otimes k} \otimes B \right) = \left(1 - \frac{k}{n} \right)^{-1} \Big(& \widetilde{A^{\otimes k}} \cdot \widetilde{B} - k \cdot \operatorname{cov}_\rho(A,B)\, \widetilde{A^{\otimes k-1}} - \frac{k}{\sqrt{n}} \operatorname{Fluct}\left(A^{\otimes k-1} \otimes (AB) \right) \\
& - \frac{k}{\sqrt{n}} \Big(\rho(A) \operatorname{Fluct}\left(A^{\otimes k-1} \otimes B \right) + \rho(B) \operatorname{Fluct}\left(A^{\otimes k} \right) \Big) \Big).
\end{aligned} \tag{3.14}$$

Hence, we obtain a recursive rule for asymptotically decomposing tensor fluctuators into elementary ones

$$\widetilde{A^{\otimes k}} = \widetilde{A^{\otimes k-1}} \cdot \widetilde{A} - (k-1) \operatorname{var}_\rho(A) \cdot \widetilde{A^{\otimes k-2}} + O\left(\frac{1}{\sqrt{n}} \right), \tag{3.15}$$

where we introduced the variance

$$\operatorname{var}_\rho(A) = \operatorname{cov}_\rho(A,A). \tag{3.16}$$

Therefore, every tensor fluctuator can be decomposed into a finite polynomial of elementary fluctuators and vice versa.

3.4. Combinatorics for product states

In this section, we compute the expectation value of products of elementary fluctuators around ρ in the product state sequence $\rho^{\otimes n}$. The two following propositions will be the basis for most proofs in the subsequent sections.

Proposition 3.4.1. *Let $\rho \in \mathcal{S}(\mathcal{A})$. Consider the elementary fluctuators $\widetilde{A}_1, ...\widetilde{A}_k$ around ρ, defined by $A_1, ..., A_k \in \mathcal{A}$, such that $\rho \cdot A_i \neq 0$ for all i. Then, using the notation $\underline{A_i} = A_i - \rho(A_i)\mathbb{1}$,*

$$\rho^{\otimes n}\big(\widetilde{A}_1 \cdot ... \cdot \widetilde{A}_k\big) = \begin{cases} \sum \rho(\underline{A}_{i_1}\underline{A}_{j_1})\rho(\underline{A}_{i_2}\underline{A}_{j_2})...\rho(\underline{A}_{i_l}\underline{A}_{j_l}) + O\left(\frac{1}{n}\right), & k \text{ even} \\ \frac{1}{\sqrt{n}} \sum \rho(\underline{A}_{i_1}\underline{A}_{j_1}\underline{A}_{h_1})\rho(\underline{A}_{i_2}\underline{A}_{j_2})...\rho(\underline{A}_{i_l}\underline{A}_{j_l}) + O\left(n^{-\frac{3}{2}}\right), & k \text{ odd,} \end{cases} \tag{3.17}$$

where in the even case, the sum goes over all pairwise decompositions $(i_1 < j_1), (i_2 < j_2), ..., (i_l < j_l)$ of the set $\{1, 2, ..., k\}$ with $l = k/2$ and in the odd case over all decompositions $(i_1 < j_1 < h_1), (i_2 < j_2), ..., (i_l < j_l)$ of the set $\{1, 2, ..., k\}$ with $l = (k-1)/2$, such that no term appears twice.

Proof. On the one hand, due to the product rule (2.7),

$$\begin{aligned} \mathrm{sym}_n A \cdot \mathrm{sym}_n(B_1 \otimes ...B_y) = &\left(1 - \frac{y}{n}\right)\mathrm{sym}_n(A \otimes B_1 \otimes ...B_y) \\ &+ \frac{y}{n}\,\mathrm{sym}_n\big(A \otimes \mathbb{1}^{\otimes y-1} \cdot \mathrm{sym}_y(B_1 \otimes ...B_y)\big). \end{aligned} \tag{3.18}$$

Hence, we can write the product of fluctuators, $\widetilde{A}_1 \cdot ... \cdot \widetilde{A}_k$ as a sum of strictly symmetric sequences, scaled with $n^{k/2}$. Each symmetric sequence, that contains overlaps of the operators $\underline{A}_i$, i.e. tensor factors of the form $... \otimes (\underline{A}_i \cdot \underline{A}_j \cdot ...) \otimes ...$, stemming from the second term on the r.h.s of (3.18), is multiplied with a factor n^{-x}, where x is the number of overlaps. Each symmetric sequence can be evaluated by

$$\rho^{\otimes n}(\mathrm{sym}_n(B_1 \otimes ... \otimes B_y)) = \rho(B_1) \cdot ... \cdot \rho(B_y). \tag{3.19}$$

Since $\rho(\underline{A}_i) = \rho(A_i) - \rho(A_i) = 0$, every strictly symmetric sequence, that contains a tensor factor $... \otimes \underline{A}_i \otimes ...$, vanishes in the expectation with $\rho^{\otimes n}$. Hence, the non-vanishing terms in (3.17) are those for which each tensor factor is either a product of several $\underline{A}_i$'s or the identity. Due to the factor $n^{k/2}$ from the fluctuators, the leading order terms are those with $x = k/2$ or $x = (k+1)/2$ overlaps, depending on whether k is even or odd. The others vanish in the limit as $O(1/n)$. If k is even, the leading-order terms are such that every tensor factor is a product of two operators, i.e. $\underline{A}_i \cdot \underline{A}_j$, with i and j such that the non-commutativity of the A_i is respected. If k is odd, then the leading-order terms contain one tensor factor with three operators, $\underline{A}_i \cdot \underline{A}_j \cdot \underline{A}_h$ and vanish as $1/\sqrt{n}$. □

Furthermore, consider $X \in \mathcal{A}$, such that $\rho X = X\rho = 0$. Then any expectation value containing $\widetilde{X}$ vanishes by the following proposition.

Proposition 3.4.2. *Consider $\rho \in \mathcal{S}(\mathcal{A})$ and the elementary fluctuators $\widetilde{A}_1, \ldots, \widetilde{A}_k$ around ρ, as in Prop. 3.4.2. Moreover, consider a fluctuator $\widetilde{X}$ with $\rho X = X\rho = 0$. If k is even, then, using the notation $\underline{A_i} = A_i - \rho(A_i)\mathbb{1}$,*

$$\rho^{\otimes n}\left(\widetilde{A}_1 \cdot \ldots \cdot \widetilde{X} \cdot \ldots \cdot \widetilde{A}_k\right) = \frac{1}{\sqrt{n}} \sum \rho(\underline{A}_{i_1} X \underline{A}_{j_1})\rho(\underline{A}_{i_2}\underline{A}_{j_2})\ldots\rho(\underline{A}_{i_l}\underline{A}_{j_l}) + O\left(n^{-\frac{3}{2}}\right), \quad (3.20)$$

where the sum goes over all pairwise decompositions $(i_1 < j_1), (i_2 < j_2), \ldots, (i_l < j_l)$ of the set $\{1, 2, \ldots, k\}$ with $l = k/2$ and i_1 less then the position of X and j_1 greater than that. If k is odd, then the expectation value amounts to

$$\begin{aligned}\rho^{\otimes n}\left(\widetilde{A}_1 \cdot \ldots \cdot \widetilde{X} \cdot \ldots \cdot \widetilde{A}_k\right) = \frac{1}{n} \sum \Big(&\rho(\underline{A}_{i_1}\underline{A}_{j_1}\underline{A}_{h_1})\rho(\underline{A}_{i_2} X \underline{A}_{j_2})\ldots\rho(\underline{A}_{i_l}\underline{A}_{j_l}) \\ &+\rho(\underline{A}_{i_1} X \underline{A}_{j_1}\underline{A}_{h_1})\rho(\underline{A}_{i_2}\underline{A}_{j_2})\ldots\rho(\underline{A}_{i_l}\underline{A}_{j_l}) \\ &+\rho(\underline{A}_{i_1}\underline{A}_{j_1} X \underline{A}_{h_1})\rho(\underline{A}_{i_2}\underline{A}_{j_2})\ldots\rho(\underline{A}_{i_l}\underline{A}_{j_l})\Big) + O\left(n^{-2}\right)\end{aligned} \quad (3.21)$$

where the sum goes over all decompositions $(i_1 < j_1 < h_1), (i_2 < j_2), \ldots, (i_l < j_l)$ of the set $\{1, 2, \ldots, k\}$ with $l = (k-1)/2$ and with i_1 less and j_1 greater (resp. j_1 and h_1 in the third line) than the position of X.

Proof. The proof is the same as for Prop. 3.4.1, but with the difference that all terms vanish, which contain the product $X\rho$ or ρX, for example

$$\rho(X\underline{A}_i) = \mathrm{Tr}(\rho X \underline{A}_i) = 0. \quad (3.22)$$

Hence in the non-vanishing terms the operator X is in a tensor factor of the form $\ldots \otimes \underline{A}_i X \underline{A}_j \otimes \ldots$ or $\ldots \otimes \underline{A}_i X \underline{A}_j \underline{A}_h \otimes \ldots$, depending on k. □

3.5. Sequences with root-n fluctuations and the limiting fluctuation algebra

In this section, we define sequences of states ρ_n, for which the expectation values with fluctuators converge. Moreover, we give an algebraic description of the corresponding limits. The results are closely related to earlier works in this direction [52, 42], but the permutation invariance allows for a more precise description. A part of the results was already presented in [111].

Definition 3.5.1. *A sequence of n-particle states $\rho_n \in \mathcal{S}(\mathcal{A}_n)$ has root-n fluctuations around ρ, if for any product of elementary fluctuators $\widetilde{A}_1, \widetilde{A}_2, \ldots$ around ρ, the limit*

$$\lim_{n\to\infty} \rho_n\left(\widetilde{A}_1\widetilde{A}_2\ldots\right) = \left\langle \Omega, \widehat{A}_1\widehat{A}_2\ldots\Omega \right\rangle \quad (3.23)$$

exists. The values of the limits are written in terms of a Hilbert space $\mathcal{H}_\rho$, such that the sequence ρ_n is identified with the unit vector $\Omega \in \mathcal{H}_\rho$ and the fluctuators $\widetilde{A}_i$ with limiting fluctuators $\widehat{A}_i$, being operators on $\mathcal{H}_\rho$. The scalar product on $\mathcal{H}_\rho$ is defined by

$$\left\langle \widehat{B}_1\ldots\widehat{B}_l\,\Omega, \widehat{A}_1\ldots\widehat{A}_k\Omega \right\rangle = \lim_{n\to\infty} \rho_n\left(\widetilde{B}_l^*\ldots\widetilde{B}_1^*\widetilde{A}_1\ldots\widetilde{A}_k\right), \quad (3.24)$$

where the elements $\widehat{A}_1\ldots\widehat{A}_k\,\Omega$ span a dense subset of $\mathcal{H}_\rho$.

The definition can equivalently be written with tensor fluctuators, cf. Def. 3.2.2, due to the decomposition rule (3.15). Since the definition asserts the existence of the limits for all products of fluctuators, we can write them as expectation values themselves, using the GNS representation [18]. The Hilbert space $\mathcal{H}_\rho$ is then by definition the closure of the span of all elements $\widehat{A}_1...\widehat{A}_k\,\Omega$. The positivity of the scalar product follows from the positivity of the states ρ_n. That is, if $\widetilde{F}$ is a polynomial of elementary fluctuators with n-independent coefficients, then $\|\widehat{F}\Omega\|^2 = \lim_n \rho_n\big(\widetilde{F}^*\widetilde{F}\big) \geq 0$.

By Prop. 3.4.1, the sequence $\rho^{\otimes n}$ has root-n fluctuations around ρ. More generally, we construct sequences with root-n fluctuations around ρ by what we call the *filtering construction*: Consider a polynomial $\widetilde{F}$ of elementary fluctuators with n-independent coefficients. Then the sequence ρ_n^F, defined by

$$\rho_n^F(X) = \frac{\rho^{\otimes n}(\widetilde{F}^* X \widetilde{F})}{\rho^{\otimes n}(\widetilde{F}^*\widetilde{F})} \quad \forall X \in \mathcal{A}_n, \tag{3.25}$$

has root-n fluctuations around ρ. Moreover the limiting vector amounts to

$$\Omega^F = \frac{\widehat{F}\Omega}{\|\widehat{F}\Omega\|}, \tag{3.26}$$

where Ω is the limiting vector for $\rho^{\otimes n}$. Hence, by definition, the set of vectors Ω^F is dense in $\mathcal{H}_\rho$, such that by the filtering construction every element of $\mathcal{H}_\rho$ can be approximated arbitrarily well. The limiting fluctuators $\widehat{A}$ around ρ, for $A \in \mathcal{A}$, generate an algebra of operators, which we denote by $\mathcal{F}_\rho$.

Lemma 3.5.2. *The fluctuation algebra $\mathcal{F}_\rho$ is an algebra of canonical commutation relations and the commutator of two fluctuators amounts to*

$$\big[\widehat{A}, \widehat{B}\big] = \rho\big([A, B]\big)\mathbb{1}. \tag{3.27}$$

Proof. Consider the vectors, $\widehat{A}_1...\widehat{A}_k\Omega$ and $\widehat{B}_1...\widehat{B}_l\Omega$, from $\mathcal{H}_\rho$, where Ω is the limiting vector of $\rho^{\otimes n}$. Moreover, let $k+l$ be even, such that the following object is non-zero. The matrix element of the commutator $\big[\widehat{A}, \widehat{B}\big]$ with these two vectors amounts to

$$\begin{aligned} &\big\langle \Omega, \widehat{B}_l^*...\widehat{B}_1^*\,\big[\widehat{A}, \widehat{B}\big]\,\widehat{A}_1...\widehat{A}_k\,\Omega\big\rangle \\ &= \lim_{n\to\infty} \rho^{\otimes n}\left(\widetilde{B}_l^*...\widetilde{B}_1^*\,\big[\widetilde{A}, \widetilde{B}\big]\,\widetilde{A}_1...\widetilde{A}_k\right) \\ &= \lim_{n\to\infty} \sum \rho\big([A, B]\big)\rho(\underline{C}_{i_1}\underline{C}_{j_1})\rho(\underline{C}_{i_2}\underline{C}_{j_2})...\rho(\underline{C}_{i_l}\underline{C}_{j_l}) \\ &= \rho\big([A, B]\big)\big\langle \Omega, \widehat{B}_l^*...\widehat{B}_1^*\widehat{A}_1...\widehat{A}_k\,\Omega\big\rangle, \end{aligned} \tag{3.28}$$

where the sums go over all elements $\underline{C}_{i_1}$, chosen either from $\{\underline{B}_i^*\}_{i=1}^l$ or $\{\underline{A}_i\}_{i=1}^k$, respecting their order in the first line. The terms containing factors $\rho(\underline{C}_{i_1}\underline{A})\rho(\underline{B}\,\underline{C}_{j_1})$ or $\rho(\underline{C}_{i_1}\underline{B})\rho(\underline{A}\,\underline{C}_{j_1})$ cancel each other in the sum. Hence, only the terms with the factor $\rho\big([A, B]\big)$ remain, and by pulling this factor out of the sum the last line follows. Since the vectors $\widehat{A}_1\widehat{A}_2...\Omega$ span a dense subset, the statement can be extended to all of $\mathcal{H}_\rho$. □

The limiting vector Ω of the sequence $\rho^{\otimes n}$ is a Gaussian state. Indeed, for all $A \in \mathcal{A}$, the characteristic function amounts to

$$\begin{aligned}
\left\langle \Omega, \exp\left(i\,\widehat{A}\right)\,\Omega \right\rangle &= \lim_{n\to\infty} \rho^{\otimes n}\left(\exp\left(i\,\widetilde{A}\right)\right) \\
&= \lim_{n\to\infty} \rho\left(\exp\left(\frac{i(A-\rho(A)\mathbb{1})}{\sqrt{n}}\right)\right)^n \\
&= \lim_{n\to\infty} \rho\left(\mathbb{1} + \frac{i(A-\rho(A)\mathbb{1})}{\sqrt{n}} - \frac{(A-\rho(A)\mathbb{1})^2}{2n}\right)^n \\
&= \exp\left(-\frac{1}{2}\mathrm{var}_\rho(A)\right).
\end{aligned} \tag{3.29}$$

This fact is also known as a non-commutative central limit theorem [42, 57, 111].

In the following, we introduce the concept of scaled fluctuators. Prop. 3.4.2 implies that $\widehat{X} = 0$, whenever $X\rho = \rho X = 0$, for $X \in \mathcal{A}$. Also, it implies that the rate, at which a related finite-n expectation value vanishes, amounts to $1/\sqrt{n}$. Hence, we can consider the limits of expectation values containing the operators $\sqrt{n}\widetilde{X}$, for $X\rho = \rho X = 0$, which we call scaled fluctuators. These are a special instance of the class of so-called abnormal fluctuators [113].

Proposition 3.5.3 (Definition and properties of scaled fluctuators)**.** *Consider $X \in \mathcal{A}$, such that $\rho X = X\rho = 0$. Then there exists an operator $\widehat{\widehat{X}} \in \mathcal{F}_\rho$, such that*

$$\lim_{n\to\infty} \rho^{\otimes n}\left(\widetilde{A}_1 ... \widetilde{A}_k \cdot \sqrt{n}\widetilde{X} \cdot \widetilde{B}_1 ... \widetilde{B}_l\right) = \left\langle \Omega,\, \widehat{A}_1 ... \widehat{A}_k \cdot \widehat{\widehat{X}} \cdot \widehat{B}_1 ... \widehat{B}_l\,\Omega \right\rangle \tag{3.30}$$

for all $\widetilde{A}_1, ..., \widetilde{A}_k, \widetilde{B}_1, ..., \widetilde{B}_l$. Moreover, $\widehat{X} = 0$ and $\widehat{\widehat{X}}$ is a quadratic operator with the commutation relation

$$\left[\widehat{\widehat{X}}, \widehat{A}\right] = \widehat{[X, A]} \quad \forall A \in \mathcal{A}. \tag{3.31}$$

Proof. The convergence of the expectation value (3.30) follows from Prop. 3.4.2 and defines $\widehat{\widehat{X}}$ on a dense subset of $\mathcal{H}_\rho$. Also, from Prop. 3.4.2 follows $\widehat{X} = 0$. The commutation relation of $\widehat{\widehat{X}}$ follows from

$$\begin{aligned}
\left[\sqrt{n}\widetilde{X}, \widetilde{A}\right] &= n\sqrt{n} \cdot \left[\mathrm{sym}_n X, \mathrm{sym}_n\left(A - \rho(A)\mathbb{1}\right)\right] \\
&= \sqrt{n}\,\mathrm{sym}_n[X, A] \\
&= \widetilde{[X, A]},
\end{aligned} \tag{3.32}$$

where the second line follows from the product rule (2.7) and the fact that $\rho X = X\rho = 0$. In the third line, we wrote the operator as a fluctuator, which is possible because $\rho([X, A]) = 0$. Since the fluctuation algebra is CCR and $\widehat{A}$ as well as $\widehat{[X, A]}$ are elementary fluctuators and thus linear in the canonical variables, it follows from (3.31) that $\widehat{\widehat{X}}$ is quadratic in the canonical variables. □

Finally, filtered sequences have the following property for finite n.

Lemma 3.5.4. *Consider a filtered sequence ρ_n^F around ρ defined by (3.25) with limiting vector Ω^F. Furthermore, consider a product of elementary fluctuators $\widetilde{A}_1$, ..., $\widetilde{A}_k$, such that some of the related operators fulfill $\rho \cdot A_i = A_i \cdot \rho = 0$, say for $1 \le i \le r$. Then*

$$\rho_n^F\big(\sqrt{n}\widetilde{A}_1 \cdot \ldots \cdot \sqrt{n}\widetilde{A}_r \cdot \widetilde{A}_{r+1} \cdot \ldots \cdot \widetilde{A}_k\big) = \Big\langle \Omega^F,\ \widehat{\widehat{A}}_1 \cdot \ldots \cdot \widehat{\widehat{A}}_r \cdot \widehat{A}_{r+1} \cdot \ldots \cdot \widehat{A}_k\, \Omega^F \Big\rangle + O\left(\frac{1}{\sqrt{n}}\right). \quad (3.33)$$

for all $n \ge k$.

Proof. Using (3.25), we can apply Prop. 3.4.1 and 3.4.2 to prove the statement. Note that in general, $\widetilde{F}$ is a polynomial of elementary fluctuators. Hence, the terms $\widetilde{F}^* \cdot \widetilde{A}_1 \cdot \ldots \cdot \widetilde{A}_k \cdot \widetilde{F}$ are a sum of products of an even number of elementary fluctuators and products of an odd number of elementary fluctuators. Therefore, the leading order is in general $O(1)$, independent of k, and the next order is in general $O(1/\sqrt{n})$. □

3.6. Normal modes and related structure

In this section, we identify the normal modes of the fluctuation algebra $\mathcal{F}_\rho$ as well as central elements and scaled fluctuators. Let $\{|k\rangle, k = 0, .., d-1\}$ be an orthonormal basis of the one-particle Hilbert space $\mathcal{H}$, such that the reference state ρ of $\mathcal{F}_\rho$ is diagonal. We denote matrix elements by $e_{kl} = |k\rangle\langle l| \in \mathcal{B}(\mathcal{H})$. The related elementary, limiting and scaled fluctuators will be denoted by $\widetilde{e_{kl}}$, $\widehat{e_{kl}}$ and $\widehat{\widehat{e_{kl}}}$, respectively.

Proposition 3.6.1. *Let $\mathcal{H}$ be a d-dimensional Hilbert space and $\rho \in \mathcal{S}(\mathcal{B}(\mathcal{H}))$ a state with rank r. Let $\big\{|k\rangle, k = 0, .., d-1\big\}$ be an orthonormal basis of $\mathcal{H}$, such that $\rho = p_0 |0\rangle\langle 0| + \ldots + p_{r-1} |r-1\rangle\langle r-1|$, with $p_0 \ge p_1 \ge \ldots \ge p_{r-1}$. Then the fluctuation algebra $\mathcal{F}_\rho$ with reference state ρ has the following structure:*

- *For $k < r$ and $k < l \le d-1$, the ladder operators a_{kl}, a_{kl}^* of the mode (k, l) amount to*

$$a_{kl} = \frac{\widehat{e_{kl}}}{\sqrt{p_k - p_l}}, \qquad a_{kl}^* = \frac{\widehat{e_{lk}}}{\sqrt{p_k - p_l}}, \quad (3.34)$$

  as long as $p_k \neq p_l$. In the case $p_k = p_l$, the related fluctuators $\widehat{e_{kl}}$ and $\widehat{e_{lk}}$ become central elements of the algebra.

- *For $k \ge r$ and $l \ge r$, $\widehat{e_{kl}} = 0$ and the related scaled fluctuator amounts to*

$$\widehat{\widehat{e_{kl}}} = \sum_{x=0}^{r-1} a_{xk}^* a_{xl}. \quad (3.35)$$

- *The diagonal elements $\widehat{e_{kk}}$ for $k < r$ are central, i.e. commute with the rest of the algebra. Moreover, they fulfill the relation*

$$\sum_{k=0}^{r-1} \widehat{e_{kk}} = 0, \ \text{and} \quad (3.36)$$

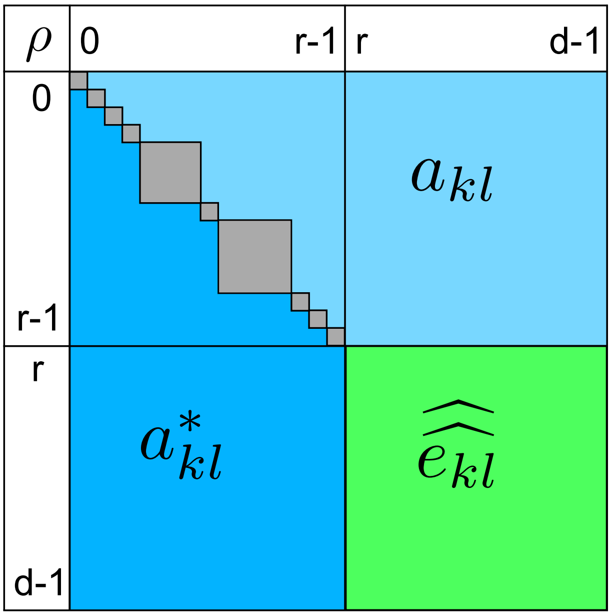

Figure 3.1.: Illustration of the normal modes of the fluctuation algebra $\mathcal{F}_\rho$, for a reference state ρ with rank r, in terms of the fluctuators $\widehat{e_{kl}}$ for $e_{kl} = |k\rangle\langle l|$, where $\{|k\rangle, k = 0,..,d-1\}$ is an orthonormal basis, such that ρ is diagonal, with the non-zero eigenvalues arranged in the first r diagonal elements in decreasing order. The matrix elements in the light blue area correspond to lowering operators a_{kl} (3.34) of $\mathcal{F}_\rho$. The ones in the dark blue area to the related raising operators. The matrix elements in the grey area correspond to central elements of $\mathcal{F}_\rho$. These are the first r diagonal elements, corresponding to the non-zero eigenvalues of ρ, and, if some eigenvalues of ρ are degenerate, the elements in the surrounding boxes as well. The matrix elements in the green area correspond to scaled fluctuators $\widehat{\widehat{e_{kl}}}$, which are quadratic operators in a_{kl} and a^*_{kl} (3.35).

$$\widehat{\widehat{\left(\sum_{k=0}^{r-1} e_{kk}\right)}} = -\sum_{k=r}^{d-1} \widehat{\widehat{e_{kk}}}. \tag{3.37}$$

The statement of this proposition is visualized in Fig. 3.1.

Proof. We start with the diagonal terms $\widehat{e_{kk}}$. These are central elements, since

$$\left[\widehat{e_{kk}}, \widehat{A}\right] = \rho\big([e_{kk}, A]\big)\mathbb{1} = \mathrm{Tr}\big([\rho, e_{kk}] \cdot A\big)\mathbb{1} = 0 \tag{3.38}$$

for any $A \in \mathcal{B}(\mathcal{H})$. Moreover, for $k \geq r$ the related fluctuators vanish, i.e. $\widehat{e_{kk}} = 0$ by Prop. 3.5.3, since $e_{kk} \cdot \rho = \rho \cdot e_{kk} = 0$. By the decomposition of the identity,

$$\sum_{k=0}^{d-1} \widetilde{e_{kk}} = \widetilde{\mathbb{1}} = \sqrt{n}\,\mathrm{sym}_n\big(\mathbb{1} - \rho(\mathbb{1})\mathbb{1}\big) = 0 \quad \forall n, \tag{3.39}$$

it follows that also the following sum vanishes,

$$\sum_{k=0}^{r-1} \widehat{e_{kk}} = 0. \tag{3.40}$$

However, the single terms $\widehat{e_{kk}}$ are non-zero for $k < r$, as we show in the following. Let $\Omega \in \mathcal{H}_\rho$ be the limiting vector of the sequence $\rho^{\otimes n}$, cf. Def 3.5.1. Then $\mathcal{H}_\rho$ is spanned by the vectors $\Psi = \widehat{A}_1 \ldots \widehat{A}_x \, \Omega$ for any monomial of fluctuators $\widehat{A}_i$. Since $\widehat{e_{kk}}$ is central, it is sufficient to evaluate the following matrix elements, which by Prop. 3.4.1 amount to

$$\begin{aligned} \langle \Psi, \widehat{e_{kk}}\, \Omega \rangle &= \left\langle \Omega, \widehat{A}_1 \ldots \widehat{A}_x \, \widehat{e_{kk}}\, \Omega \right\rangle \\ &= \sum_{i, i_1, j_1, i_2 \ldots} \rho\big(A_i \cdot \big(e_{kk} - p_k \mathbb{1}\big)\big) \cdot \rho(A_{i_1} A_{j_1}) \cdot \ldots + O\left(\frac{1}{n}\right). \end{aligned} \tag{3.41}$$

Here, we assume $\rho(A_i) = 0$ for all i. Each term in the leading order of (3.41) contains a factor

$$\rho\big(A_i \cdot \big(e_{kk} - p_k \mathbb{1}\big)\big) = p_k\big(\langle k|\, A_i \,|k\rangle - \rho(A_i)\big), \tag{3.42}$$

which is non-zero in general. Next, we consider the fluctuators of non-diagonal matrix elements. The commutator of two of these amounts to

$$\begin{aligned} \left[\widehat{e_{kl}}, \widehat{e_{ij}}\right] &= \rho\big([e_{kl}, e_{ij}]\big) \mathbb{1} \\ &= (p_k - p_l) \delta_{il} \delta_{jk} \mathbb{1}. \end{aligned} \tag{3.43}$$

Therefore, provided that $p_k - p_l \neq 0$, we can identify the lowering operators of the fluctuation algebra by

$$a_{kl} = \frac{\widehat{e_{kl}}}{\sqrt{p_k - p_l}}, \quad k \in \{0, .., r-1\},\, k < l \in \{1, .., d-1\} \tag{3.44}$$

and the raising operators as their conjugates. If $p_k = p_l$, then the related fluctuators $\widehat{e_{kl}}$ and $\widehat{e_{lk}}$ become central elements of the algebra (3.43). Moreover, since $\rho(A \cdot e_{kl}) = p_k \langle k|\, A \,|l\rangle$, these elements are non-zero (3.41).

Finally, we describe the scaled fluctuators of the algebra and their decomposition into ladder operators. The scaled fluctuators are given by $\widehat{\widehat{e_{kl}}}$ for $k, l \geq r$, since $e_{kl} \cdot \rho = \rho \cdot e_{kl} = 0$, cf. Prop 3.4.2. Furthermore, this implies that

$$\widehat{\widehat{\left(\sum_{k=0}^{r-1} e_{kk}\right)}} = -\sum_{k=r}^{d-1} \widehat{\widehat{e_{kk}}}, \tag{3.45}$$

such that the sum of the diagonal matrix elements e_{kk}, $k = 0, \ldots, r-1$ defines a scaled fluctuator as well. Note, that in this case the condition of Prop. 3.4.2 is not fulfilled, that is

$$\rho \cdot \sum_{k=0}^{r-1} e_{kk} = \rho \cdot \mathbb{1} \neq 0. \tag{3.46}$$

However, considering Eq. (3.17), we see that

$$\rho\left(A \cdot \sum_{k=0}^{r-1}\big(e_{kk} - \rho(e_{kk})\big)\mathbb{1}\right) = \rho(A) - \rho(A) = 0. \tag{3.47}$$

Hence, the leading order in Eq. (3.17) vanishes. However, the operators $\widehat{\widehat{e_{kk}}}$ themselves are not defined for $k < r$. For $k, l \geq r$, the commutator of $\widehat{\widehat{e_{kl}}}$ with a fluctuator amounts to

$$\begin{aligned}\left[\widehat{\widehat{e_{kl}}},\, \widehat{e_{ij}}\right] &= \widehat{\left[e_{kl},\, e_{ij}\right]} \\ &= \widehat{e_{kj}}\delta_{li} - \widehat{e_{il}}\delta_{kj},\end{aligned} \tag{3.48}$$

by Prop. 3.5.3. Moreover,

$$\begin{aligned}\left\langle \Psi,\, \widehat{\widehat{e_{kl}}}\,\Omega\right\rangle &= \lim_{n\to\infty} \rho^{\otimes n}\left(\widetilde{X_1}\ldots\widetilde{X_s} \cdot \sqrt{n}\widetilde{e_{kl}}\right) \\ &= \sum_{\alpha} n^{-\frac{\alpha}{2}} \rho(\ldots) \cdot \ldots \cdot \rho\left(\ldots \cdot \sqrt{n} e_{kl}\right) = 0,\end{aligned} \tag{3.49}$$

since $e_{lk} \cdot \rho = 0$. Eq. (3.49) outrules a part proportional to $\mathbb{1}$ in $\widehat{\widehat{e_{kl}}}$. Therefore, using the definition of the ladder operators, we can write

$$\begin{aligned}\widehat{\widehat{e_{kl}}} &= \sum_{x=0}^{r-1} \frac{1}{p_x} \widehat{e_{kx}}\,\widehat{e_{xl}} \\ &= \sum_{x=0}^{r-1} a_{xk}^* a_{xl}.\end{aligned} \tag{3.50}$$

The probabilities p_x cancel out, because $p_k = p_l = 0$. □

Remark 3.6.2. *For $k \geq r$, the basis of the subspace* span$\{|k\rangle\}$ *is not uniquely defined by ρ. Hence, one can choose an arbitrary orthonormal basis $\{|k'\rangle\}$ for that subspace, and always get the above structure of the fluctuation algebra for the related matrix elements.*

Remark 3.6.3. *The total number of modes, $M(\rho)$, amounts to*

$$M(\rho) = r\left(d - \frac{r+1}{2}\right) - \Delta, \tag{3.51}$$

where $d = \dim \mathcal{H}$, $r = rank(\rho)$ and Δ amounts to the number of modes that are eliminated due to degeneracy of the eigenvalues of ρ.

Remark 3.6.4. *If ρ is not pure, then the related fluctuation state $|\Omega\rangle$ is not the vacuum state. For example, the particle number in the* 01*-mode amounts to*

$$\begin{aligned}\langle \Omega,\, a_{01}^* a_{01}\,\Omega\rangle &= \frac{1}{p_0 - p1}\rho\big(|1\rangle\langle 0| \cdot |0\rangle\langle 1|\big) \\ &= \frac{p_1}{p_0 - p_1}.\end{aligned} \tag{3.52}$$

4. First-order corrections to the mean-field ground-state energy

4.1. Overview

In this chapter, we describe a method for obtaining $1/n$-corrections to the ground-state energy of a strictly symmetric Hamiltonian density $H_n = \mathrm{sym}_n H_k$, using the concept of mean-field fluctuations. In section 4.2, we introduce the essential idea, which is to find the mean-field ground state ρ_0, minimizing H_∞, and to consider the fluctuation algebra $\mathcal{F}_{\rho_0}$ around it. We introduce an expansion of H_n into fluctuators in $\mathcal{F}_{\rho_0}$. While the mean-field minimum amounts to the evaluation $\rho_0^{\otimes n}(H_n)$, the expansion into fluctuators allows us to minimize H_n over sequences ρ_n with root-n fluctuations around ρ_0, i.e. beyond product states. We obtain an asymptotic expansion of the expectation value $\rho_n(H_n)$, where the zeroth (constant) order is given by the mean-field ground-state energy and the first order in $1/n$ by the expectation value of a suitable *fluctuation Hamiltonian* $\widehat{H}$ in the limiting vector $\Omega \in \mathcal{H}_{\rho_0}$ of the sequence ρ_n. Hence, in order to estimate the ground-state energy of H_n up to order $1/n$ from above, it suffices to find the ground-state energy of the related fluctuation Hamiltonian $\widehat{H}$. We state the ground-state energy estimation as an inequality, because we cannot show that the true $1/n$ corrections can be attained in this way in general. That is, in other words, we cannot show that the sequence of true ground states of H_n satisfies the root-n fluctuation property. A preliminary result of this method was already presented in [111], namely the expansion of H_n into fluctuators, and an estimation was given for the special case of ρ_0 being in the interior of the state space, i.e. of full rank.

In Section 4.3, we reduce the method to systems that contain Bose symmetry, i.e. allowing only states ρ_n that are supported only on the Bose sector, cf. Eq. (2.55). We show that, in order to do so, it suffices to restrict the minimization of H_∞ to the submanifold of pure states, hence finding the pure state with lowest H_∞-value. In particular, it is not necessary for this state to be a minimizer on the full state space. We obtain upper and lower bounds on the ground-state energy of $\widehat{H}$, which directly correspond to the second derivatives of H_∞ on the pure submanifold at the minimizer.

In Section 4.4, we lift these bounds to full mean-field models, i.e. those allowing all permutation invariant states, by showing that such models can be embedded into Bosonic mean-field models using purification techniques.

In sections 4.5, 4.6 and 4.7, we apply the mean-field ground-state estimation method to three cases. Firstly, we consider the mean-field Ising model, cf. Eq. (2.18) and obtain analytical expressions for the $1/n$-corrections to the ground-state energy. Secondly, we consider the Bose-Hubbard model and show for the one-dimensional case that the fluctuation Hamiltonian is exactly the well-known Bogoliubov Hamiltonian. We outline some aspects of the physics of the Bose-Hubbard model and discuss the difference between the mean-field limit and the thermodynamic limit. Thirdly, we apply the ground-state estimation to the finite de Finetti theorem, cf. Thm. 2.5.3, and show that our method provides an inner version of a finite de Finetti bound.

In Section 4.8, we relate the fluctuation method to the widely used Holstein-Primakoff approximation, showing that the latter is a special case of the former.

Finally, in Section 4.9, we propose an extension of the ground-state estimation method to a class of approximately symmetric Hamiltonian densities, which contains a wide range of physically interesting models, such as the Lipkin-Meshkov-Glick model or the Bose-Hubbard model without the artifical mean-field scaling, cf. Section 4.6.

4.2. The ground-state energy estimation method

Throughout this chapter, and as in most of the previous chapters, let $\mathcal{A} = \mathcal{B}(\mathcal{H})$ be the operator algebra for one quantum particle with $\dim(\mathcal{H}) = d$, and $\mathcal{A}_n \in \mathcal{A}^{\otimes n}$ the algebra of permutation invariant n-particle operators. We consider a mean-field quantum system with a strictly symmetric Hamiltonian density, $H_n = \mathrm{sym}_n H_k$. The mean-field function H_∞ of that Hamiltonian density is therefore a polynomial of degree k. In the following, we utilize the method of mean-field fluctuations to estimate the ground-state energy of H_n up to order $1/n$. Due to the Taylor expansion (2.41), we can write H_n as

$$H_n = \sum_{r=0}^{k} \frac{1}{r!} \mathrm{sym}_n\big(\mathrm{d}_r H_\infty(\rho)\big) \quad \forall \rho \in \mathcal{S}(\mathcal{A}). \tag{4.1}$$

Since the derivatives have the property $\rho \otimes \sigma^{\otimes r-1}\big(\mathrm{d}_r H_\infty(\rho)\big) = 0$ by Def. 2.4.2, we can write the Hamiltonian density in terms of the fluctuators $\widetilde{\mathrm{d}_r H_\infty}(\rho) = n^{r/2}\mathrm{d}_r H_\infty(\rho)$, i.e.

$$H_n = \sum_{r=0}^{k} \frac{1}{r!} n^{-\frac{r}{2}} \widetilde{\mathrm{d}_r H_\infty}(\rho) \quad \forall \rho \in \mathcal{S}(\mathcal{A}). \tag{4.2}$$

Hence, the expectation value with an arbitrary n-particle state ρ_n amounts to

$$\rho_n(H_n) = H_\infty(\rho) + \frac{1}{\sqrt{n}}\rho_n\big(\widetilde{\mathrm{d}H_\infty}(\rho)\big) + \frac{1}{2n}\rho_n\big(\widetilde{\mathrm{d}_2 H_\infty}(\rho)\big) + \dots \quad \forall \rho \in \mathcal{S}(\mathcal{A}). \tag{4.3}$$

Note that for general sequences ρ_n, the terms $\rho_n\big(\widetilde{\mathrm{d}_r H_\infty}(\rho)\big)$ may diverge in the limit $n \to \infty$. However, if the sequence ρ_n has root-n fluctuations around ρ, then Eq. (4.3) gives rise to an asymptotic expansion, in the sense that $\rho_n\big(\widetilde{\mathrm{d}_r H_\infty}(\rho)\big)$ only contributes to the orders $n^{-r/2}$ and lower in (4.3). Our Ansatz is to minimize $\rho_n(H_n)$ over sequences with root-n fluctuations. For this, we choose the reference state to be $\rho = \rho_0$, a minimizer of H_∞, hence minimizing the leading-order term in (4.3). Then we consider ρ_n as a sequence with root-n fluctuations around ρ_0, such that we write (4.3) as an asymptotic series, where we are only interested in the terms up to order $1/n$. Since ρ_0 is a minimizer, there are two possibilities for the gradient and the Hessian of H_∞. If ρ_0 is in the interior of $\mathcal{S}(\mathcal{A})$, i.e. has full rank, then $\mathrm{d}H_\infty(\rho_0) = 0$ and $\mathrm{d}_2 H_\infty(\rho_0) \geq 0$. If ρ_0 is located on the boundary of $\mathcal{S}(\mathcal{A})$, then the gradient need not vanish, but must to be positive in each allowed direction, hence $\mathrm{d}H_\infty(\rho_0) \geq 0$. Moreover, $\rho_0 \cdot \mathrm{d}H_\infty(\rho_0) = \mathrm{d}H_\infty(\rho_0) \cdot \rho_0 = 0$ by Lem. 4.2.1. The Hessian can in this case have positive and negative eigenvalues.

Lemma 4.2.1. *Let $\rho \in \mathcal{S}(\mathcal{A})$ be a minimizer of the differentiable function $f \in \mathcal{C}(\mathcal{S}(\mathcal{A}))$. Then $\rho \cdot \mathrm{d}f(\rho) = \mathrm{d}f(\rho) \cdot \rho = 0$.*

Proof. As a density matrix, ρ is positive, i.e. $\rho \geq 0$. Since ρ is a minimizer, $\mathrm{d}f(\rho) \geq 0$, too. Define A and B by $\rho = A^*A$ and $\mathrm{d}f(\rho) = B^*B$. By Def. 2.4.1,

$$\rho(\mathrm{d}f(\rho)) = \mathrm{Tr}\big(\rho \cdot \mathrm{d}f(\rho)\big) = \mathrm{Tr}(A^*AB^*B) = \mathrm{Tr}((BA^*)^* \cdot BA^*) = 0. \tag{4.4}$$

Define $C = BA^*$. Then C^*C is positive, and since $\mathrm{Tr}(C^*C) = 0$ by (4.4), $C = 0$. That is, $BA^* = AB^* = 0$ and thus $\rho \cdot \mathrm{d}f(\rho) = \mathrm{d}f(\rho) \cdot \rho = 0$. □

The following theorem is the general statement of the ground-state estimation of H_n up to order $1/n$.

Theorem 4.2.2. *Let $\mathcal{A} = \mathcal{B}(\mathcal{H})$ with $\dim \mathcal{H} = d$, and $H_n \in \mathcal{A}_n$ a strictly symmetric sequence. Then its ground-state energy $\min H_n$ is, up to order $1/n$, upper bounded by*

$$\min H_n \leq H_\infty(\rho_0) + \frac{1}{n} \inf \widehat{H} + O\left(n^{-\frac{3}{2}}\right), \tag{4.5}$$

where ρ_0 is a minimizer of H_∞ and $\inf \widehat{H}$ is the ground-state energy of the fluctuation Hamiltonian

$$\widehat{H} = \widehat{\widehat{\mathrm{d}H_\infty}}(\rho_0) + \frac{1}{2}\widehat{\mathrm{d}_2 H_\infty}(\rho_0) \in \mathcal{F}_{\rho_0} \tag{4.6}$$

around ρ_0. Moreover, $\widehat{H}$ is a quadratic Hamiltonian with $\inf \widehat{H}$ finite and non-positive.

Proof. Consider a sequence ρ_n with root-n fluctuations around some ρ. Then the expectation value $\rho_n(H_n)$ can be written in terms of the fluctuator expansion (4.3). Minimizing the reference state ρ with respect to H_∞ minimizes the zeroth order of the expansion. Minimizing over all sequences ρ_n with root-n fluctuations around a H_∞–minimizer ρ_0 then minimizes the next order. Note that $\rho_0 \cdot \mathrm{d}H_\infty(\rho_0) = \mathrm{d}H_\infty(\rho_0) \cdot \rho_0 = 0$ by Lem. 4.2.1, hence $\mathrm{d}H_\infty(\rho_0)$ gives rise to a scaled fluctuator. We consider sequences ρ_n^F, that are constructed by the filtering construction (3.25) with some polynomial $\widetilde{F}$ of fluctuators around the minimizer ρ_0. By Lem. 3.5.4, we obtain the following expansion for such sequences:

$$\begin{aligned} \rho_n^F(H_n) &= H_\infty(\rho_0) + \frac{1}{n}\rho_n^F\left(\sqrt{n}\widehat{\mathrm{d}H_\infty}(\rho_0) + \frac{1}{2}\widehat{\mathrm{d}_2 H_\infty}(\rho_0)\right) + O\left(n^{-\frac{3}{2}}\right) \\ &= H_\infty(\rho_0) + \frac{1}{n}\left\langle \Omega^F, \widehat{H}\,\Omega^F \right\rangle + O\left(n^{-\frac{3}{2}}\right). \end{aligned} \tag{4.7}$$

Since the set of filtered limiting states Ω^F is dense in $\mathcal{H}_{\rho_0}$, it suffices to find the ground-state energy of $\widehat{H}$ in order to obtain (4.5). $\widehat{H}$ is quadratic by definition and its ground-state energy, $\inf \widehat{H}$, must be non-positive, because there exists a vector Ω with $\langle \Omega, \widehat{H}\,\Omega \rangle = 0$, namely the limiting vector of the sequence $\rho_0^{\otimes n}$. The finiteness of $\inf \widehat{H}$ is shown by applying the purification, Prop. 4.4.7, which maps the problem to a Bosonic one (See section 4.3) and then applying Thm. 4.3.3. □

Remark 4.2.3. *The minimizer ρ_0 of H_∞ need not be unique. In that case* (4.5) *holds for all minimizers and the best bound can be obtained by optimizing over all minimizers. In Example 4.2.5, a Hamiltonian density with different $1/n$-corrections for different minimizers is presented.*

Remark 4.2.4. *Eq.* (4.5) *can only serve as an upper bound, because the set of sequences ρ_n with root-n fluctuations around a mean-field minimizer ρ_0 are not directly related to the true ground states of H_n for finite n. That is, for any fixed n, consider the set of states ρ_n, that minimize H_n. We call these the true ground states[1]. The question is, does there exist a sequence (in n) of true ground states ρ_n, that has root-n fluctuations around a minimizer of H_∞? If yes, then the inequality* (4.5) *can be updated to an equality. However, a proof of this statement seems to require techniques not considered in this thesis. In Cor. 4.4.8 below, we state that this problem can be reduced to a Bosonic one.*

Example 4.2.5. *In the following, we construct an example of a system with a degenerate mean-field minimizer, where each minimizer leads to different $1/n$-corrections. Consider the 4-qubit Hamiltonian*

$$H_4 = (\sigma_x \otimes \sigma_x + \sigma_y \otimes \sigma_y) \otimes \sigma_z \otimes \sigma_z \tag{4.8}$$

and the related strictly symmetric sequence $H_n = \mathrm{sym}_n H_4$. Parametrizing 1-particle states $\rho \in \mathcal{S}(\mathcal{A})$ by the Pauli-expectation values $(x, y, z) = (\rho(\sigma_x), \rho(\sigma_y), \rho(\sigma_z))$, we can write the mean-field limiting function as

$$H_\infty(x, y, z) = (x^2 + y^2) \cdot z^2. \tag{4.9}$$

This function has a wide range of minimizers, all leading to $\inf H_\infty = 0$. We consider a subset of the minimizers, parametrized by $\rho_z \cong (0, 0, z)$ with $z \geq 0$. For these states, the gradient vanishes, i.e. $\mathrm{d}H_\infty(\rho_z) = 0$, and Hessian amounts to

$$\mathrm{d}_2 H_\infty(\rho_z) = 2z^2 \cdot (\sigma_x \otimes \sigma_x + \sigma_y \otimes \sigma_y), \tag{4.10}$$

since $\rho_z(\sigma_x) = \rho_z(\sigma_y) = 0$. Hence, only the Hessian contributes to the fluctuator expansion (4.3)*. Using* (3.15),

$$\widetilde{\sigma_x \otimes \sigma_x} = \widetilde{\sigma}_x^2 - \mathbb{1}_n + O\left(\frac{1}{\sqrt{n}}\right), \tag{4.11}$$

[1] Of course, for a given n-particle Hamiltonian density H_n, there need not be a unique minimizer ρ_n.

we obtain $\widehat{\sigma_x \otimes \sigma_x} = \widehat{\sigma}_x^2 - \mathbb{1}$, *and* $\widehat{\sigma_y \otimes \sigma_y} = \widehat{\sigma}_y^2 - \mathbb{1}$. *Moreover, by the commutator* $\left[\widehat{\sigma}_x, \widehat{\sigma}_y\right] = 2iz\mathbb{1}$, *cf. Eq.* (3.27)*, we can identify the position and momentum operators by* $Q = \widehat{\sigma}_x/\sqrt{2z}$ *and* $P = \widehat{\sigma}_y/\sqrt{2z}$*, for* $z > 0$*. Hence, the fluctuation Hamiltonian at* ρ_z *can be written as*

$$\widehat{H}_z = \frac{1}{2}\widehat{\mathrm{d}_2 H_\infty}(\rho_z) = 2z^3\big(Q^2 + P^2\big) - 2z^2\mathbb{1}, \tag{4.12}$$

and its ground-state energy amounts to

$$\inf \widehat{\mathrm{d}_2 H_\infty}(\rho_z) = -2(1-z)z^2. \tag{4.13}$$

Being this the $1/n$*-coefficient for the estimation of the ground-state energy of the Hamiltonian density* H_n*, cf. Eq.* (4.5)*, we see the dependence on the choice of the mean-field minimizer.*

In the subsequent sections, we will show that $\inf \widehat{H}$ is always finite and below zero. In Section 4.3, we will restrict the problem to Bosonic particles and obtain bounds for $\inf \widehat{H}$. In Section 4.4, we will consider the full case and show that it can be mapped into a Bosonic problem by purification, such that the related bounds for $\inf \widehat{H}$ hold in this case as well.

4.3. Ground-state-energy corrections restricted to Bosons

A research field in which mean-field methods are frequently used, is Bose-Einstein condensation [69, 85]. In fact, due to the indistinguishability of the particles, Bosonic systems contain the permutation invariance by definition. Hence, it seems straightforward to apply the mean-field and fluctuations method to such systems[2]. In this section, we show that the ground-state energy and the related $1/n$-corrections of Bosonic systems can be obtained with the mean-field and fluctuations method by simply restricting to pure states on the one-particle state space.

The definition of a Bose-symmetric n-particle state $\rho_n \in \mathcal{S}(\mathcal{A}^{\otimes n})$ is that it is not just invariant under permutations, i.e. commutes with unitaries U_π that implement permutations, $[U_\pi, \rho_n] = 0$, but even invariant under multiplication of those, i.e. $U_\pi \rho = \rho$ for all $\pi \in \mathcal{S}_n$. In other words, the density matrix ρ_n is only supported by symmetric vectors $|\psi_n\rangle \in \mathcal{H}^{\otimes n}$, which fulfill $U_\pi |\psi_n\rangle = |\psi_n\rangle$ for all $\pi \in \mathcal{S}_n$, cf. Section 2.5.

In the mean-field limit, it means that we consider Bose-symmetric states Φ on the inductive limit algebra[3] $\mathcal{A}^\infty = \overline{\bigcup_n \mathcal{A}_n}$. By Størmer's de Finetti theorem [109], for every permutation invariant state Φ on $\mathcal{A}^\infty$, there exists a probability measure μ on $\mathcal{S}(\mathcal{A})$, such that $\rho_n = \int \mathrm{d}\mu\, \rho^{\otimes n}$ for all n, cf. Prop. 2.5.2. Bose symmetry is given, if and only if μ is only supported on the pure states of the one-particle state space, by Lem. 4.3.1. In other words, we consider Bose symmetry in the mean-field limit exactly by considering only the submanifold of pure states, $\mathcal{S}_{\mathrm{pure}}(\mathcal{A}) \subset \mathcal{S}(\mathcal{A})$.

[2] However, this does not mean, that every Bosonic Hamiltonian is automatically strictly symmetric, cf. Section 4.6.2.

[3] The correspondence between permutation invariant states on $\mathcal{A}^\infty$ and states on the mean-field algebra was shown in [31].

Lemma 4.3.1 ([54])**.** *Let $\mathcal{A}$ be a finite dimensional matrix algebra. The n-particle state $\rho^{\otimes n} \in \mathcal{S}(\mathcal{A})^{\otimes n}$ is Bosonic if and only if ρ is pure.*

If we consider sequences with root-n fluctuations around a pure reference $\sigma = |\psi\rangle\langle\psi| \in \mathcal{S}_{\text{pure}}(\mathcal{A})$, the question arises, how to restrict these to Bosonic states. The answer is relatively simple: Since we consider only the corresponding limiting vectors $\Omega \in \mathcal{H}_\sigma$ for the ground-state energy estimation, cf. Eq. (4.5), we need to minimize the fluctuation Hamiltonian $\widehat{H}$ only over those vectors in $\mathcal{H}_\sigma$, that are limiting vectors of Bosonic sequences ρ_n with root-n fluctuations around σ. By Lem. 4.3.2, the sequences σ_n^F that are obtained by the filtering construction, cf. Eq. (3.25), are Bosonic sequences. By Def. 3.5.1, the related limiting vectors Ω^F are dense in $\mathcal{H}_\sigma$. That is, if the reference state $\sigma \in \mathcal{S}(\mathcal{A})$ is pure, then there exists a dense subset of the fluctuation Hilbert space $\mathcal{H}_\sigma$, that corresponds to Bosonic sequences with root-n fluctuations around σ.

Lemma 4.3.2. *Let $\mathcal{A}$ be a finite dimensional matrix algebra. The permutation invariant n-particle state ρ_n^F defined by*

$$\rho_n^F(X) = \frac{\rho^{\otimes n}\left(\widetilde{F^*}X\widetilde{F}\right)}{\rho^{\otimes n}\left(\widetilde{F^*}\widetilde{F}\right)} \quad \forall X \in \mathcal{A}^{\otimes n}, \tag{4.14}$$

with $\widetilde{F}$ being an arbitrary polynomial of fluctuators around ρ, is Bosonic if and only if ρ is pure.

Proof. We can equivalently define the density matrix

$$\rho_n^F = \frac{\widetilde{F}\rho^{\otimes n}\widetilde{F^*}}{\operatorname{Tr}\left(\widetilde{F}\rho^{\otimes n}\widetilde{F^*}\right)}. \tag{4.15}$$

In the Schur-Weyl decomposition, cf. Eq. (2.55), the state $\rho^{\otimes n}$ amounts to

$$\rho^{\otimes n} = \bigoplus_Y w_{\rho^{\otimes n},Y} \cdot \frac{\mathbb{1}_{\mathcal{H}_Y}}{\dim \mathcal{H}_Y} \otimes \left(\rho^{\otimes n}\right)_{\mathcal{H}_Y}, \tag{4.16}$$

where the sum goes over all Young diagrams Y of the n-particle permutation group S_n and $\mathcal{H}_Y$ is the corresponding irreducible representation space of the group and $\mathcal{K}_Y$ the related multiplicity space. $\rho^{\otimes n}$ is Bosonic by definition, iff the weight $w_{\rho^{\otimes n},Y}$ is one for the Bosonic subspace, cf. Eq. (2.56), and zero for all others. By Lem. 4.3.1, this is the case if and only if ρ is pure. The polynomials $\widetilde{F}$ are permutation invariant n-particle operators as well and therefore allow for the same kind of Schur-Weyl block diagonalization, cf. Eq. (2.54). Hence, multiplication of $\rho^{\otimes n}$ with these does not change the weights $w_{\rho^{\otimes n},Y}$. Therefore, ρ_n^F has the same weights as $\rho^{\otimes n}$ and thus is Bosonic if and only if ρ is pure. □

Therefore, in order to restrict the ground-state energy estimation method to Bosonic states, it suffices to merely restrict the mean-field limit to pure one-particle states $\sigma \in \mathcal{S}_{\text{pure}}(\mathcal{A})$. The ground-state energy of the corresponding fluctuation Hamiltonian $\widehat{H}$ then automatically satisfies the Bose symmetry in the sense that there exist Bose-symmetric sequences ρ_n that approximate the ground-state energy of $\widehat{H}$ arbitrarily well.

In the following subsections, we restrict the ground-state estimation method to the submanifold of pure states, $\mathcal{S}_{\mathrm{pure}}(\mathcal{A})$. The main difference to the full method, which was introduced in the previous section, is that the gradient $\mathrm{d}H_\infty(\sigma)$ need not be positive semi-definite at a pure minimum $\sigma \in \mathcal{S}_{\mathrm{pure}}(\mathcal{A})$, since the function H_∞ may decrease towards the interior of $\mathcal{S}(\mathcal{A})$. In Section 4.3.1, we derive a set of conditions for σ to be a minimum on $\mathcal{S}_{\mathrm{pure}}(\mathcal{A})$. Furthermore, we show that $\mathrm{d}H_\infty(\sigma)$ actually contributes to the fluctuation Hamiltonian in terms of a second-order effect along the submanifold $\mathcal{S}_{\mathrm{pure}}(\mathcal{A})$ due to the curvature.

In Section 4.3.2, we derive the related fluctuation Hamiltonian $\widehat{H}$ and show that it admits $1/n$-corrections. More precisely, in Thm. 4.3.3, we prove bounds on the ground-state energy of $\widehat{H}$ that are exactly derived from the condition of $\sigma \in \mathcal{S}_{\mathrm{pure}}(\mathcal{A})$ being a minimum on the pure submanifold.

Finally, in Section 4.3.3, we consider the case of Spin-$\frac{1}{2}$ particles, and obtain a particularly simple form for the fluctuation Hamiltonian and its ground-state energy.

4.3.1. Minimizing functions over pure states

The set of pure states $\mathcal{S}_{\mathrm{pure}}(\mathcal{A}) \subset \mathcal{S}(\mathcal{A})$, which is a symplectic submanifold (cf. Section 2.4) can be parametrized by unitary evolutions

$$\sigma_t = e^{-iAt}\sigma e^{iAt} \tag{4.17}$$

of some pure state $\sigma = |\psi\rangle\langle\psi|$, with $t \in \mathbb{R}$ and $A = A^* \in \mathcal{A}$.

Consider a twice differentiable function $f \in \mathcal{C}(\mathcal{S}(\mathcal{A}))$. The point $\sigma = |\psi\rangle\langle\psi|$ is a local minimum of f on the pure submanifold, if for every $A = A^* \in \mathcal{A}$, the two conditions

$$\frac{\mathrm{d}}{\mathrm{d}t} f(\sigma_t)\Big|_{t=0} = \dot{\sigma}(\mathrm{d}f(\sigma)) = 0 \qquad \text{and} \tag{4.18}$$

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2} f(\sigma_t)\Big|_{t=0} = \ddot{\sigma}(\mathrm{d}f(\sigma)) + \dot{\sigma}^{\otimes 2}(d_2 f(\sigma)) \geq 0 \tag{4.19}$$

hold, where

$$\dot{\sigma} = |\dot{\psi}\rangle\langle\psi| + |\psi\rangle\langle\dot{\psi}| \quad \text{and} \tag{4.20}$$

$$\ddot{\sigma} = |\ddot{\psi}\rangle\langle\psi| + |\psi\rangle\langle\ddot{\psi}| + 2|\dot{\psi}\rangle\langle\dot{\psi}| \tag{4.21}$$

with $|\dot{\psi}\rangle = iA|\psi\rangle$ and $|\ddot{\psi}\rangle = -A^2|\psi\rangle$. In the following, we write simply $\mathrm{d}f$ and $\mathrm{d}_2 f$ instead of $\mathrm{d}f(\sigma)$ and $\mathrm{d}_2 f(\sigma)$. The conditions (4.18) and (4.19) lead to restrictions on them. On the one hand, (4.18) can only be fulfilled for all $\dot{\psi} \perp \psi$, if

$$\mathrm{d}f\ |\psi\rangle = 0. \tag{4.22}$$

Note that $\langle\psi, \mathrm{d}f\,\psi\rangle = 0$ by Def. 2.39. However, $\mathrm{d}f$ need not be a positive operator, since f may decrease towards the interior of $\mathcal{S}(\mathcal{A})$. With (4.22), the condition for the second derivative (4.19) amounts to

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2} f(\sigma_t)\Big|_{t=0} = 2\,\mathrm{Re}\left\langle \psi\dot{\psi}\right| \mathrm{d}_2 f \left|\psi\dot{\psi}\right\rangle + 2\,\mathrm{Re}\left\langle \dot{\psi}\psi\right| \mathrm{d}_2 f \left|\psi\dot{\psi}\right\rangle + 2\left\langle \dot{\psi}\right| \mathrm{d}f \left|\dot{\psi}\right\rangle \geq 0, \tag{4.23}$$

where we simplified the notation by $|\chi\eta\rangle := |\chi \otimes \eta\rangle$ for all $\chi, \eta \in \mathcal{H}$. Since $\mathrm{d}_2 f$ is hermitian, $\left\langle \dot{\psi}\psi\right| \mathrm{d}_2 f \left|\psi\dot{\psi}\right\rangle \in \mathbb{R}$. Of particular interest are the vectors $\chi = \dot{\psi} \perp \psi$. Hence, we obtain the inequality

$$\langle\chi| \mathrm{d}f |\chi\rangle + \langle\chi\psi| \mathrm{d}_2 f |\psi\chi\rangle + \mathrm{Re}\left(e^{i\phi} \langle\psi\psi| \mathrm{d}_2 f |\chi\chi\rangle\right) \geq 0 \quad \forall \chi \perp \psi \in \mathcal{H},\ \phi \in \mathbb{R}. \tag{4.24}$$

The phase factor $e^{i\phi}$ follows from the fact that if $\chi \perp \psi$ is a valid derivative of ψ, then so is $e^{i\phi}\chi$ for all $\phi \in \mathbb{R}$, cf. Eq. (4.17).

4.3.2. Minimizing the fluctuation Hamiltonian

We consider now the fluctuations around the pure minimum $\sigma = |\psi\rangle\langle\psi| \in \mathcal{S}_{\mathrm{pure}}(\mathcal{A})$ for some twice differentiable function $f \in \mathcal{C}(\mathcal{S}(\mathcal{A}))$, which resembles the mean-field limiting Hamiltonian function and $\widehat{f} = \widehat{\widehat{\mathrm{d}f}} + \frac{1}{2}\widehat{\mathrm{d}_2 f}$ denotes the related fluctuation Hamiltonian. In this section we derive bounds on the ground-state energy of $\widehat{f}$. For this, we won't need a finite-n version $H_n \in \mathcal{A}_n$, hence it is not necessary to speak of a sequence $(H_n)_n$.

Consider an orthonormal basis $\{|0\rangle, ..., |d-1\rangle\}$ on the d-dimensional one-particle Hilbert space $\mathcal{H}$, such that $|\psi\rangle = |0\rangle$. We denote matrix elements by $e_{kl} = |k\rangle\langle l|$ in this basis. By Thm. 3.6.1, the fluctuation algebra at ψ is spanned by the ladder operators

$$a_k = \widehat{e_{0k}} \quad \text{and} \tag{4.25}$$

$$a_k^* = \widehat{e_{k0}} \quad \text{for } k = 1, ..., d-1, \tag{4.26}$$

whereas $\widehat{e_{kl}} = 0$ and $\widehat{\widehat{e_{kl}}} = a_k^* a_l$ for all other e_{kl}. In the following, we will use the decomposition rules for tensor fluctuators (3.15), i.e.

$$\begin{aligned} \widehat{e_{kl} \otimes e_{mn}} &= \widehat{e_{kl}} \cdot \widehat{e_{mn}} - (\delta_{k0}\delta_{lm}\delta_{n0} - \delta_{k0}\delta_{l0}\delta_{m0}\delta_{n0})\mathbb{1} \\ &= \begin{cases} a_k^* a_m^* & , k \neq 0, l = 0, m \neq 0, n = 0 \\ a_k^* a_n & , k \neq 0, l = 0, m = 0, n \neq 0 \\ a_l a_m^* - \delta_{lm}\mathbb{1} & , k = 0, l \neq 0, m \neq 0, n = 0 \\ a_l a_n & , k = 0, l \neq 0, m = 0, n \neq 0 \\ 0 & , \text{else} \end{cases} \end{aligned} \tag{4.27}$$

The third case can also be written as $a_l a_m^* - \delta_{lm}\mathbb{1} = a_m^* a_l$. The fluctuation Hamiltonian therefore amounts to

$$\begin{aligned}
\widehat{f} &= \widehat{\widehat{\mathrm{d}f}} + \frac{1}{2}\widehat{\mathrm{d}_2 f} \\
&= \sum_{k,l=0}^{d-1} \langle k|\,\mathrm{d}f\,|l\rangle\, \widehat{\widehat{e_{kl}}} + \frac{1}{2}\sum_{k,l,m,n=0}^{d-1} \langle km|\,\mathrm{d}_2 f\,|ln\rangle\, \widehat{e_{kl}\otimes e_{mn}} \\
&= \sum_{k,l=1}^{d-1} \big(\langle k|\,\mathrm{d}f\,|l\rangle + \langle k0|\,\mathrm{d}_2 f\,|0l\rangle\big) a_k^* a_l + \frac{1}{2}\sum_{k,l=1}^{d-1}\big(\langle 00|\,\mathrm{d}_2 f\,|kl\rangle\, a_k a_l + \langle kl|\,\mathrm{d}_2 f\,|00\rangle\, a_k^* a_l^*\big) \\
&= \sum_{k,l=1}^{d-1} D_{kl} a_k^* a_l + \frac{1}{2}\sum_{k,l=1}^{d-1}\big(C_{kl} a_k a_l + \overline{C_{kl}} a_k^* a_l^*\big) \\
&= \begin{pmatrix}\mathbf{a}^* & \mathbf{a}\end{pmatrix}\begin{pmatrix} D & \frac{1}{2}C^* \\ \frac{1}{2}C & 0\end{pmatrix}\begin{pmatrix}\mathbf{a} \\ \mathbf{a}^*\end{pmatrix} \\
&= \frac{1}{2}\begin{pmatrix}\mathbf{a}^* & \mathbf{a}\end{pmatrix}\begin{pmatrix} D & C^* \\ C & D^T\end{pmatrix}\begin{pmatrix}\mathbf{a} \\ \mathbf{a}^*\end{pmatrix} - \frac{1}{2}\operatorname{Tr}(D)\mathbb{1},
\end{aligned} \tag{4.28}$$

where in the third line we used $\langle 0k|\,\mathrm{d}_2 f\,|l0\rangle = \langle k0|\,\mathrm{d}_2 f\,|0l\rangle$ due to permutation invariance, and in the fifth line $\mathbf{a} = (a_1, ..., a_k)$. In the last line, we used the canonical commutation relations to bring the quadratic form into a standard one, Cf. [51]. Furthermore, we introduced the matrices D and C with

$$D_{kl} = \langle k|\,\mathrm{d}f\,|l\rangle + \langle k0|\,\mathrm{d}_2 f\,|0l\rangle \quad \text{and} \tag{4.29}$$

$$C_{kl} = \langle 00|\,\mathrm{d}_2 f\,|kl\rangle\,, \tag{4.30}$$

fulfilling $D = D^*$ and $C = C^T$, resp. $\overline{C} = C^*$. Moreover, D can be identified with the one-particle operator, which we in abuse of notation denote by D as well, by

$$\begin{aligned}
D &= \sum_{k,l=0}^{d-1} D_{kl} e_{kl} \\
&= \mathrm{d}f + \mathrm{id}\otimes\sigma\big(\mathrm{d}_2 f\cdot\mathbb{F}\big),
\end{aligned} \tag{4.31}$$

where $\mathbb{F} = \sum_{k,l=0}^{d-1} e_{kl}\otimes e_{lk}$ is the flip operator. The following theorem ensures that $\widehat{f}$ is bounded from below and has a negative ground-state energy.

Theorem 4.3.3. *Let $\mathcal{A} = \mathcal{B}(\mathcal{H})$ with $\dim\mathcal{H} = d$. Let $f \in \mathcal{C}(\mathcal{S}(\mathcal{A}))$ be twice differentiable at $\sigma = |\psi\rangle\langle\psi| \in \mathcal{S}(\mathcal{A})$ and σ be a local minimum on the pure submanifold such that* (4.18) *and* (4.19) *hold. Then the fluctuation Hamiltonian $\widehat{f} = \widehat{\widehat{\mathrm{d}f}} + \frac{1}{2}\widehat{\mathrm{d}_2 f}$ at σ has a ground-state energy E_0, that lies in the range*

$$-\frac{1}{2}\operatorname{Tr}\big(\mathrm{d}f + \mathrm{id}\otimes\sigma(\mathrm{d}_2 f\cdot\mathbb{F})\big) \le E_0 \le 0. \tag{4.32}$$

Proof. W.l.o.g., define an orthonormal basis $\{|0\rangle, ..., |d-1\rangle\}$ on the d-dimensional one-particle Hilbert space $\mathcal{H}$, such that $|\psi\rangle = |0\rangle$. We use the notation given in the beginning of this section, to write

$$\widehat{f} = \frac{1}{2}\begin{pmatrix}\mathbf{a}^* & \mathbf{a}\end{pmatrix}\begin{pmatrix}D & C^* \\ C & D^T\end{pmatrix}\begin{pmatrix}\mathbf{a} \\ \mathbf{a}^*\end{pmatrix} - \frac{1}{2}\operatorname{Tr}(D)\mathbb{1}. \tag{4.33}$$

In particular, $D = \mathrm{d}f + \mathrm{id} \otimes \sigma(\mathrm{d}_2 f \cdot \mathbb{F})$, cf. Eq. (4.31), such that in the statement of the theorem the lower bound for the energy is given by $-\frac{1}{2}\operatorname{Tr}(D)$, which is just the shift in $\widehat{f}$.

First, we prove the left inequality of (4.32). This requires $\widehat{f}$ to be a harmonic oscillator with non-negative frequencies. This is exactly the case [51], if

$$\begin{pmatrix}D & C^* \\ C & D^T\end{pmatrix} \geq 0. \tag{4.34}$$

Consider D and C as matrices on the Hilbert space $\mathbb{C}^d$, with the scalar product $\langle x, y\rangle = \sum_{kl} \overline{x}_k y_l$. Then the positivity in (4.34) is equivalent to the positivity of all expectation values with vectors $|z\rangle = |x\rangle \oplus |\overline{y}\rangle \in \mathbb{C}^{2d}$, where we used the complex conjugate of the vector $|y\rangle$ for convenience. That is,

$$\begin{aligned}&\begin{pmatrix}\langle x| & \langle \overline{y}|\end{pmatrix}\begin{pmatrix}D & C^* \\ C & D^T\end{pmatrix}\begin{pmatrix}|x\rangle \\ |\overline{y}\rangle\end{pmatrix} \\ &= \langle x| D |x\rangle + \langle \overline{y}| D^T |\overline{y}\rangle + 2\operatorname{Re}\langle \overline{y}| C |x\rangle \\ &= \langle x| D |x\rangle + \langle y| D |y\rangle + \operatorname{Re}\langle \Psi_C |(xy + yx)\rangle \geq 0,\end{aligned} \tag{4.35}$$

where $xy = x \otimes y$ and $\langle \Psi_C |xy\rangle := \langle \overline{y}| C |x\rangle = \langle 00| \mathrm{d}_2 f |xy\rangle$. Obviously, $\mathcal{H} \cong \mathbb{C}^d$, such that we can consider the vectors x and y as elements of $\mathcal{H}$. The positivity of (4.35) is fulfilled if and only if (4.24) is fulfilled. We use (4.24) with two different phase factors ϕ.

$$\langle \chi| D |\chi\rangle + \operatorname{Re}\langle \Psi_C |\chi\chi\rangle \geq 0 \quad \text{and} \tag{4.36}$$

$$\langle \gamma| D |\gamma\rangle - \operatorname{Re}\langle \Psi_C |\gamma\gamma\rangle \geq 0 \quad \forall \chi, \gamma \perp \psi. \tag{4.37}$$

The sum of the two equations amounts to

$$\begin{aligned}&\langle \chi| D |\chi\rangle + \langle \gamma| D |\gamma\rangle + \operatorname{Re}\langle \Psi_C |(\chi\chi - \gamma\gamma)\rangle \\ &= \langle x| D |x\rangle + \langle y| D |y\rangle + \operatorname{Re}\langle \Psi_C |(xy + yx)\rangle \geq 0 \quad \forall \chi, \gamma \perp \psi,\end{aligned} \tag{4.38}$$

where in the second line we defined $x = \frac{1}{\sqrt{2}}(\chi + \gamma)$ and $y = \frac{1}{\sqrt{2}}(\chi - \gamma)$ and used the polarization identity

$$2(A \otimes A \pm B \otimes B) = (A + B) \otimes (A \pm B) + (A - B) \otimes (A \mp B) \quad \forall A, B \in \mathcal{H}. \tag{4.39}$$

Hence, the left inequality of (4.32) is proven.

Next, we prove the right inequality of (4.32), i.e. that $\widehat{f}$ cannot have a positive ground-state energy. For this, it is convenient to switch to the position/momentum representation, by defining

$$Q_k = \frac{1}{\sqrt{2}}\left(a_k + a_k^*\right) \quad \text{and} \tag{4.40}$$

$$P_k = -\frac{i}{\sqrt{2}}\left(a_k - a_k^*\right) \quad \forall k. \tag{4.41}$$

In this representation, the fluctuation Hamiltonian has the form

$$\begin{aligned}\widehat{f} &= \frac{1}{4}\begin{pmatrix}\mathbf{Q} & \mathbf{P}\end{pmatrix}\begin{pmatrix} D + D^T + C + C^* & i\left(D - D^T + C - C^*\right) \\ -i\left(D - D^T - C + C^*\right) & D + D^T - C - C^*\end{pmatrix}\begin{pmatrix}\mathbf{Q} \\ \mathbf{P}\end{pmatrix} - \frac{1}{2}\operatorname{Tr}(D)\mathbb{1} \\ &= \begin{pmatrix}\mathbf{Q'} & \mathbf{P'}\end{pmatrix}\begin{pmatrix}\omega & 0 \\ 0 & \omega\end{pmatrix}\begin{pmatrix}\mathbf{Q'} \\ \mathbf{P'}\end{pmatrix} - \frac{1}{2}\operatorname{Tr}(D)\mathbb{1},\end{aligned} \tag{4.42}$$

where $\mathbf{Q} = (Q_1, ..., Q_{d-1})$, $\mathbf{P} = (P_1, ..., P_{d-1})$ and $\mathbf{Q'}$ and $\mathbf{P'}$ accordingly. In the second line we applied Prop. 4.3.5, to perform a symplectic diagonalization with $\omega = \operatorname{diag}(\omega_1, ..., \omega_{d-1})$ and $\omega_i \geq 0$. Clearly, the ground-state energy of $\widehat{f}$ is the sum of the frequencies minus the shift, that is

$$E_0 = \operatorname{Tr}(\omega) - \frac{1}{2}\operatorname{Tr}(D). \tag{4.43}$$

Since

$$\frac{1}{4}\operatorname{Tr}\begin{pmatrix} D + D^T + C + \overline{C} & i\left(D - D^T + C - \overline{C}\right) \\ -i\left(D - D^T - C + \overline{C}\right) & D + D^T - C - \overline{C}\end{pmatrix} = \operatorname{Tr}(D), \tag{4.44}$$

we have $2\operatorname{Tr}(\omega) \leq \operatorname{Tr}(D)$ by Lem. 4.3.6. Hence, $E_0 \leq 0$, proving the right inequality of (4.32). □

Remark 4.3.4. *The upper bound for the ground-state energy of $\widehat{f}$, i.e.* $\inf \widehat{f} \leq 0$ *can be alternatively proved much easier, if we consider finite particle numbers n. Indeed, consider the n-particle fluctuation Hamiltonian*

$$\widetilde{f} = \sqrt{n}\,\widetilde{\mathrm{d}f}(\sigma) + \frac{1}{2}\widetilde{\mathrm{d}_2 f}(\sigma). \tag{4.45}$$

Then the trivial sequence $\sigma^{\otimes n}$ fulfills $\sigma^{\otimes n}(\widetilde{f}) = 0\,\forall n$. Hence, the related limiting vector Ω has the property $\langle\Omega, \widehat{f}\,\Omega\rangle = 0$, implying that $\inf \widehat{f} \leq 0$.

Proposition 4.3.5 (Williamson [119])**.** *Let A be a real and positive definite $2n \times 2n$-matrix. Then there exists a symplectic matrix $S \in Sp(2n, \mathbb{R})$, such that*

$$SAS^T = \operatorname{diag}(\lambda_1, ..., \lambda_n, \lambda_1, ..., \lambda_n) \tag{4.46}$$

with $\lambda_i > 0\,\forall i$.

Lemma 4.3.6. *Let* $\Omega = \begin{pmatrix} \Lambda & 0 \\ 0 & \Lambda \end{pmatrix}$ *be a* $2n \times 2n$*-dimensional matrix with* $\Lambda = \mathrm{diag}(\lambda_1, ..., \lambda_n)$ *and* $\lambda_i > 0\, \forall i$*. Then for every symplectic transformation* $S \in Sp(2n, \mathbb{R})$*,*

$$\mathrm{Tr}\left(S\Omega S^T\right) \geq \mathrm{Tr}(\Omega). \tag{4.47}$$

Proof. By the Euler or Bloch-Messiah decomposition [14, 19], every symplectic matrix S can be written using the orthogonal and symplectic matrices K and K' and the matrix $D = \mathrm{diag}(d_1, .., d_n) > 0$, which is unique up to permutations of the eigenvalues as

$$S = K' \begin{pmatrix} D & 0 \\ 0 & D^{-1} \end{pmatrix} K. \tag{4.48}$$

Therefore, using the orthogonality of K' and the cyclicity of the trace,

$$\mathrm{Tr}\left(S\Omega S^T\right) = \mathrm{Tr}\left(\begin{pmatrix} D^2 & 0 \\ 0 & D^{-2} \end{pmatrix} K\Omega K^T\right). \tag{4.49}$$

Furthermore, every orthogonal symplectic matrix K has the form

$$K = \begin{pmatrix} X & Y \\ -Y & X \end{pmatrix}, \tag{4.50}$$

where $X + iY$ is unitary [123]. We therefore obtain the equality

$$\begin{aligned} \mathrm{Tr}\left(K\Omega K^T\right) &= 2\,\mathrm{Tr}\big(X\Lambda X + Y\Lambda Y\big) \\ &= \mathrm{Tr}(\Omega) \\ &= 2\,\mathrm{Tr}(\Lambda), \end{aligned} \tag{4.51}$$

where the second line follows again from the invariance of the trace under orthogonal transformations. Therefore, the statement of the lemma is proven by

$$\begin{aligned} \mathrm{Tr}\left(S\Omega S^T\right) &= \mathrm{Tr}\left(\begin{pmatrix} D^2 & 0 \\ 0 & D^{-2} \end{pmatrix} K\Omega K^T\right) \\ &= \sum_{i=1}^{n} \left(d_1^2 + \frac{1}{d_i^2}\right) \cdot \big((X\Lambda X)_i + (Y\Lambda Y)_i\big) \\ &\geq 2 \cdot \sum_{i=1}^{n} \big((X\Lambda X)_i + (Y\Lambda Y)_i\big) \\ &= \mathrm{Tr}(\Omega), \end{aligned} \tag{4.52}$$

where $(X\Lambda X)_i$ and $(Y\Lambda Y)_i$ are the diagonal elements of $X\Lambda X$ and $Y\Lambda Y$, respectively. □

4.3.3. Spin-$\frac{1}{2}$ case

In the following, we consider the case of Spin-$\frac{1}{2}$ particles, that is, $d-2$. In this case, the matrices C and D are just numbers, i.e.

$$D = \langle 1|\,\mathrm{d}f\,|1\rangle + \langle 10|\,\mathrm{d}_2 f\,|01\rangle \tag{4.53}$$

and

$$C = \langle 00|\,\mathrm{d}_2 f\,|11\rangle\,. \tag{4.54}$$

The frequency of the harmonic oscillator (4.28) amounts to $\omega = \sqrt{D^2 - |C|^2}$, where $\pm\omega$ are the eigenvalues of

$$I\mathcal{D} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} D & \overline{C} \\ C & D \end{pmatrix}, \tag{4.55}$$

[51]. Hence, there exists a Bogoliubov transformation into ladder operators b and b^*, such that

$$\widehat{f} = \frac{1}{2}\big(\omega(b^* b + b b^*) - D \cdot \mathbb{1}\big). \tag{4.56}$$

The ground-state energy therefore amounts to

$$E_0 = \frac{1}{2}\Big(\sqrt{D^2 - |C|^2} - D\Big). \tag{4.57}$$

4.4. Ground-state-energy corrections for the full mean-field case

In this section we consider again the mean-field ground-state problem on the whole of $\mathcal{S}(\mathcal{A})$. That is, we allow the minimizer to be mixed and derive bounds for the ground-state energy of the related fluctuation Hamiltonian. We do this by mapping the problem again to a Bosonic one via purification, such that we can just apply Prop. 4.3.3.

We set up the notation as follows. As before, let $\mathcal{A} = \mathcal{B}(\mathcal{H})$ be the one-particle operator algebra, with $\dim \mathcal{H} = d$. The n-particle algebra of permutation invariant operators is denoted by $\mathcal{A}_n \subset \mathcal{A}^{\otimes n}$. A permutation automorphism is given by $A_n \mapsto \pi(A_n)$ for $\pi \in \mathcal{S}_n$ and the symmetrization map amounts to

$$\mathrm{sym}_n(A_k) = \frac{1}{n!} \sum_\pi \pi(A_k \otimes \mathbb{1}^{\otimes n-k}). \tag{4.58}$$

We introduce now what we call the extended mean-field system. Define $\mathcal{H}_p = \mathcal{H} \otimes \mathcal{K}$ with $\mathcal{K} \cong \mathcal{H}$ and $\mathcal{A}_p = \mathcal{B}(\mathcal{H}_p)$ as the one-particle algebra of the extended system. For the n-fold tensor product, we use the isomorphy

$$(\mathcal{H} \otimes \mathcal{K})^{\otimes n} \cong \mathcal{H}^{\otimes n} \otimes \mathcal{K}^{\otimes n}. \tag{4.59}$$

Throughout this section, we will represent vectors and operators of the extended system using the r.h.s. of the above equation, if not stated differently. Hence, a permutation automorphism on $\mathcal{A}_p^{\otimes n} = \mathcal{B}(\mathcal{H}^{\otimes n} \otimes \mathcal{K}^{\otimes n})$ can be written as $A_{p,n} \mapsto \pi \otimes \pi(A_{p,n})$ for $A_{p,n} \in$

$\mathcal{A}_p^{\otimes n}$, where $\pi(.)$ is a representation of $\pi \in \mathcal{S}_n$ on $\mathcal{B}(\mathcal{A}^{\otimes n})$. Therefore, we can define a symmetrization map on the extended system by

$$\mathrm{sym}_{p,n}(A_k \otimes B_k) = \frac{1}{n!} \sum_\pi \pi(A_k \otimes \mathbb{1}^{\otimes n-k}) \otimes \pi(B_k \otimes \mathbb{1}^{\otimes n-k}). \tag{4.60}$$

Definition 4.4.1. *For $A_n \in \mathcal{A}_n$, the operator*

$$A_{p,n} = A_n \otimes \mathbb{1}_n \in \mathcal{A}_{p,n}, \tag{4.61}$$

where $\mathbb{1}_n$ is the identity on $\mathcal{K}^{\otimes n}$, is called the extension of A_n.

Lemma 4.4.2. *Let $(A_n)_n$ be a strictly symmetric sequence. Then $(A_{p,n})_n$ with $A_{p,n} = A_n \otimes \mathbb{1}_n$ is strictly symmetric as well. Furthermore, if $(A_n)_n$ is approximately symmetric, then so is $(A_{p,n})_n$.*

Proof. We start with the strictly symmetric part. Let $A_n = \mathrm{sym}_n A_k$. Then

$$A_{p,n} = (\mathrm{sym}_n A_k) \otimes \mathbb{1}_n = \mathrm{sym}_{p,n}(A_k \otimes \mathbb{1}_k) = \mathrm{sym}_{p,n}(A_{p,k}). \tag{4.62}$$

On the other hand,

$$\left\| A_{p,n} - \mathrm{sym}_{p,n}(A_{p,m}) \right\| = \| A_n \otimes \mathbb{1}_n - (\mathrm{sym}_n A_m) \otimes \mathbb{1}_n \| = \| A_n - \mathrm{sym}_n A_m \| . \tag{4.63}$$

Hence, if $(A_n)_n$ is approximately symmetric, then so is $(A_{p,n})_n$ by Def. 2.2.1. □

By Lem. 4.4.2, (4.61) maps mean-field models from $\mathcal{A}_n$ to $\mathcal{A}_{p,n}$. We now take a closer look at the states on those systems. Clearly, they are related by partial traces, i.e.

$$\mathrm{Tr}\big(\rho_{p,n} \cdot (A_n \otimes \mathbb{1}_n)\big) = \mathrm{Tr}\big(\mathrm{Tr}_{\mathcal{K}^{\otimes n}}(\rho_n) \cdot A_n\big) \quad \forall \rho_{p,n} \in \mathcal{S}(\mathcal{A}_{p,n}). \tag{4.64}$$

Indeed, the map (4.61) is just the dual of the partial trace $\mathrm{Tr}_{\mathcal{K}^{\otimes n}}(.)$, where the tensor factors acting on $\mathcal{K}^{\otimes n}$ are traced out. This relation also carries over to the mean-field limiting functions, that is

$$A_{p,\infty}(\rho_p) = A_\infty\big(\mathrm{Tr}_{\mathcal{K}}(\rho_p)\big) \quad \forall \rho_p \in \mathcal{S}(\mathcal{A}_p). \tag{4.65}$$

Hence, we get the following equivalence of the ground-state problems

$$\min_{\rho_n \in \mathcal{S}(\mathcal{A}_n)} \rho_n(A_n) = \min_{\rho_{p,n} \in \mathcal{S}(\mathcal{A}_{p,n})} \rho_{p,n}(A_{p,n}) \tag{4.66}$$

and

$$\min_{\rho \in \mathcal{S}(\mathcal{A})} A_\infty(\rho) = \min_{\rho_p \in \mathcal{S}(\mathcal{A}_p)} A_{p,\infty}(\rho_p). \tag{4.67}$$

However, we are more interested in the correspondence between states $\rho_n \in \mathcal{S}(\mathcal{A}_n)$ and pure states on $\mathcal{A}_{p,n}$, which are defined by Bose-symmetric vectors $|\psi_{\rho_n}\rangle \in \mathcal{H}_p^{\otimes n}$. Indeed, this correspondence is given by purification.

Lemma 4.4.3 ([78])**.** *Let $\rho \in \mathcal{S}(\mathcal{A})$. Then there exists a vector $|\psi_\rho\rangle \in \mathcal{H}_p$, such that*

$$\rho(A) = \langle\psi_\rho| A \otimes \mathbb{1} |\psi_\rho\rangle \quad \forall A \in \mathcal{A}. \tag{4.68}$$

Such a vector is given by $|\psi_\rho\rangle = (\sqrt{\rho} \otimes \mathbb{1})|\psi\rangle$, where $|\psi\rangle = \sum_i |e_i\rangle \otimes |f_i\rangle$ and $\{|e_i\rangle\}$ and $\{|f_i\rangle\}$ are orthonormal bases on $\mathcal{H}$ and $\mathcal{K}$, respectively.

Lemma 4.4.4 ([23])**.** *Let $\rho_n \in \mathcal{S}(\mathcal{A}_n)$ be a permutation invariant state. Then there exists a Bose-symmetric vector $|\psi_{\rho_n}\rangle \in \mathcal{H}_p^{\otimes n}$, such that $\rho_n = \mathrm{Tr}_{\mathcal{K}^{\otimes n}}(|\psi_{\rho_n}\rangle\langle\psi_{\rho_n}|)$. The vector is given by*

$$|\psi_{\rho_n}\rangle = \left(\sqrt{\rho_n} \otimes \mathbb{1}_n\right)|\psi_n\rangle, \tag{4.69}$$

where

$$|\psi_n\rangle = |\psi\rangle^{\otimes n} = \left(\sum_i |e_i\rangle \otimes |f_i\rangle\right)^{\otimes n} \tag{4.70}$$

and $\{|e_i\rangle\}$ and $\{|f_i\rangle\}$ are orthonormal bases on $\mathcal{H}$ and $\mathcal{K}$, respectively.

Furthermore, if $\rho_n = \rho^{\otimes n}$, i.e. is a product state, then a purification of ρ_n is given by

$$\left|\psi_{\rho^{\otimes n}}\right\rangle = |\psi_\rho\rangle^{\otimes n} = \left((\sqrt{\rho} \otimes \mathbb{1})|\psi\rangle\right)^{\otimes n}, \tag{4.71}$$

since $\sqrt{\rho^{\otimes n}} = \sqrt{\rho}^{\otimes n}$. Thus, we get the relations

$$\rho_n(A_n) = \langle\psi_{\rho_n}| A_{p,n} |\psi_{\rho_n}\rangle \quad \forall \rho_n \in \mathcal{S}(\mathcal{A}_n), \tag{4.72}$$

$$\rho^{\otimes n}(A_n) = \left\langle\psi_\rho^{\otimes n}\right| A_{p,n} \left|\psi_\rho^{\otimes n}\right\rangle \quad \forall \rho \in \mathcal{S}(\mathcal{A}) \tag{4.73}$$

and

$$A_\infty(\rho) = A_{p,\infty}(|\psi_\rho\rangle\langle\psi_\rho|) \quad \forall \rho \in \mathcal{S}(\mathcal{A}). \tag{4.74}$$

The ground-state problem for a mean-field model on $\mathcal{A}_n$ is therefore equivalent to the Bosonic ground-state problem for the related extended model on $\mathcal{A}_{p,n}$. That is, in order to estimate the ground-state energy of a mean-field model on $\mathcal{A}_n$, it suffices to perform the Bosonic ground-state energy estimation on the extended mean-field model on $\mathcal{A}_{p,n}$.

We take now a closer look at the derivatives of the limiting functions.

Lemma 4.4.5. *If A_∞ is k times differentiable, then so is $A_{p,\infty}$, and the kth derivative amounts to*

$$\mathrm{d}_k A_{p,\infty}(\rho_p) = \mathrm{d}_k A_\infty\left(\mathrm{Tr}_{\mathcal{K}}(\rho_p)\right) \otimes \mathbb{1}_k \quad \forall \rho_p \in \mathcal{S}(\mathcal{A}_p) \tag{4.75}$$

Proof. By Def. 2.4.2

$$\begin{aligned}
\sigma_p^{\otimes k}\left(\mathrm{d}_k A_{p,\infty}(\rho_p)\right) &= \frac{\mathrm{d}^k}{\mathrm{d}\mu^k} A_{p,\infty}\left((1-\mu)\rho_p + \mu\sigma_p\right)\Big|_{\mu=0} \\
&= \frac{\mathrm{d}^k}{\mathrm{d}\mu^k} A_\infty\left((1-\mu)\rho + \mu\sigma\right)\Big|_{\mu=0} \\
&= \sigma^{\otimes k}\left(\mathrm{d}_k A_\infty(\rho)\right),
\end{aligned} \tag{4.76}$$

where $\rho = \mathrm{Tr}_{\mathcal{K}}(\rho_p)$ and $\sigma = \mathrm{Tr}_{\mathcal{K}}(\sigma_p)$. □

Moreover, the correspondence holds for all purifications ψ_ρ of ρ, i.e.

$$\mathrm{d}_k A_{p,\infty}(\psi_\rho) = \mathrm{d}_k A_\infty\big(\rho\big) \otimes \mathbb{1}_k \quad \forall \rho \in \mathcal{S}(\mathcal{A}). \tag{4.77}$$

We consider now the fluctuations of the corresponding models and show the equality of the obtained $1/n$-corrections. For a fluctuator $\widetilde{A} \in \mathcal{A}_n$ around $\rho \in \mathcal{S}(\mathcal{A})$, we define a fluctuator $\widetilde{A_p} \in \mathcal{A}_{p,n}$ around the purification $|\psi_\rho\rangle \in \mathcal{H}_p$ by

$$\begin{aligned}
\widetilde{A_p} &= \widetilde{A} \otimes \mathbb{1}_n \\
&= \sqrt{n}\big(\mathrm{sym}_n(A - \rho(A)\mathbb{1})\big) \otimes \mathbb{1}_n \\
&= \sqrt{n}\,\mathrm{sym}_{p,n}\big(A \otimes \mathbb{1} - \rho(A)\mathbb{1} \otimes \mathbb{1}\big) \\
&= \sqrt{n}\,\mathrm{sym}_{p,n}\big(A \otimes \mathbb{1} - \langle\psi_\rho| A \otimes \mathbb{1} |\psi_\rho\rangle \cdot \mathbb{1} \otimes \mathbb{1}\big) \\
&= (\widetilde{A \otimes \mathbb{1}})_p.
\end{aligned} \tag{4.78}$$

Clearly, if a sequence ρ_n has root-n fluctuations around $\rho \in \mathcal{S}(\mathcal{A})$, then for the sequence $|\psi_{\rho_n}\rangle$ of purifications, the expectation values

$$\langle\psi_{\rho_n}| \widetilde{A_p}\widetilde{B_p} \cdot \ldots |\psi_{\rho_n}\rangle = \rho_n(\widetilde{A}\widetilde{B}\ldots) \tag{4.79}$$

converge as $n \to \infty$. However, this does not imply that the sequence $|\psi_{\rho_n}\rangle$ has root-n fluctuations around $|\psi_\rho\rangle$, because there also exist fluctuators

$$(\widetilde{A \otimes B})_p = \sqrt{n}\,\mathrm{sym}_{p,n}\big(A \otimes B - \langle\psi_\rho| A \otimes B |\psi_\rho\rangle \cdot \mathbb{1} \otimes \mathbb{1}\big), \tag{4.80}$$

for which the convergence in expectation with $|\psi_{\rho_n}\rangle$ need not hold. To distinguish this, we introduce the following definition

Definition 4.4.6. *A sequence of states $\rho_{p,n} \in \mathcal{S}(\mathcal{A}_{p,n})$ is said to have restricted root-n fluctuations around $\rho_p \in \mathcal{S}(\mathcal{A}_p)$, if for all $A, B, \ldots \in \mathcal{A}$*

$$\lim_{n\to\infty} \rho_{p,n}\big(\widetilde{A_p}\widetilde{B_p}\ldots\big) = \big\langle \Omega,\, \widehat{A}\widehat{B}\ldots\Omega\big\rangle \tag{4.81}$$

exists, where $\widetilde{X_p} = \widetilde{X} \otimes \mathbb{1}_n$ for $X = A, B, \ldots$.

Proposition 4.4.7. *Consider a mean-field Hamiltonian function H_∞ with minimizer $\rho \in \mathcal{S}(\mathcal{A})$, the related extended function $H_{p,\infty}$, and the fluctuation Hamiltonians $\widetilde{H}$ around ρ and $\widetilde{H}_p$ around a purification $|\psi_\rho\rangle\langle\psi_\rho| \in \mathcal{S}(\mathcal{A}_p)$. Then*

$$\inf \widehat{H} = \inf \widehat{H}_p. \tag{4.82}$$

Proof. On the one hand, assume the sequence $\rho_{p,n}$ has root-n fluctuations around $|\psi_\rho\rangle\langle\psi_\rho|$ with $\lim_{n\to\infty} \rho_{p,n}(\widetilde{H}_p) = \big\langle \Psi_p,\, \widehat{H}_p\,\Psi_p\big\rangle$. Then it also has restricted fluctuations, by Def. 4.4.6, and the sequence $\rho_n = \mathrm{Tr}_{\mathcal{K}^{\otimes n}}(\rho_{p,n})$ has root-n fluctuations around ρ with the same limit, since

$$\rho_{p,n}(\widetilde{H}_p) = \rho_{p,n}(\widetilde{H} \otimes \mathbb{1}_n) = \rho_n(\widetilde{H}) \quad \forall n. \tag{4.83}$$

On the other hand, assume some expectation value $\langle \Psi, \widehat{H}\,\Psi \rangle \in \mathbb{R}$ of $\widehat{H}$. Then, by the filtering construction (3.25), there exists a polynomial $\widetilde{F}$ of fluctuators around ρ with n-independent coefficients, such that the related filtered sequence approximates the expectation values arbitrarily well. That is, for every $\epsilon > 0$, there exists a $\widetilde{F}$, such that

$$\left| \lim_{n\to\infty} \frac{\rho^{\otimes n}\big(\widetilde{F}\widetilde{H}\widetilde{F}^*\big)}{\rho^{\otimes n}\big(\widetilde{F}\widetilde{F}^*\big)} - \langle \Psi, \widehat{H}\,\Psi \rangle \right| \leq \epsilon. \tag{4.84}$$

The polynomial $\widetilde{F}$ defines a filtered sequence on $\mathcal{A}_{p,n}$ by purification, which implies the same expectation value on $\widehat{H}_p$. That is by Eq. (4.78),

$$\begin{aligned} \frac{\rho^{\otimes n}\big(\widetilde{F}\widetilde{H}\widetilde{F}^*\big)}{\rho^{\otimes n}\big(\widetilde{F}\widetilde{F}^*\big)} &= \frac{\langle \psi_\rho^{\otimes n} | \, (\widetilde{F \otimes \mathbb{1}})_p (\widetilde{H \otimes \mathbb{1}})_p (\widetilde{F \otimes \mathbb{1}})_p^* \, | \psi_\rho^{\otimes n} \rangle}{\langle \psi_\rho^{\otimes n} | \, (\widetilde{F \otimes \mathbb{1}})_p (\widetilde{F \otimes \mathbb{1}})_p^* \, | \psi_\rho^{\otimes n} \rangle} \\ &= \langle \psi_{\rho,n}^F | \, \widetilde{H}_p \, | \psi_{\rho,n}^F \rangle \quad \forall n \end{aligned} \tag{4.85}$$

and therefore

$$\begin{aligned} &\left| \lim_{n\to\infty} \frac{\rho^{\otimes n}\big(\widetilde{F}\widetilde{H}\widetilde{F}^*\big)}{\rho^{\otimes n}\big(\widetilde{F}\widetilde{F}^*\big)} - \langle \Psi, \widehat{H}\,\Psi \rangle \right| \\ = &\left| \lim_{n\to\infty} \langle \psi_{\rho,n}^F | \, \widetilde{H}_p \, | \psi_{\rho,n}^F \rangle - \langle \Psi, \widehat{H}\,\Psi \rangle \right| \\ = &\left| \langle \Psi_p^F, \widehat{H}_p \, \Psi_p^F \rangle - \langle \Psi, \widehat{H}\,\Psi \rangle \right| \leq \epsilon. \end{aligned} \tag{4.86}$$

□

Hence, it follows that the ground state of a fluctuation Hamiltonian $\widehat{H}$ is always finite and non-positive, since Thm. 4.3.3 applies to the fluctuation Hamiltonian $\widehat{H}_p$ of the extended model. We close this section with the following corollary on sequences of true ground states of H_n.

Corollary 4.4.8. *Assume, a sequence of true ground states ρ_n of H_n has root-n fluctuations around a mean-field minimizer ρ of H_∞, cf. Rem. 4.2.4. Then every sequence of purifications $|\psi_{\rho_n}\rangle\langle\psi_{\rho_n}|$ of ρ_n has restricted root-n fluctuations around the purification $|\psi\rangle\langle\psi|$ of ρ, by Eq.* (4.79)*, and the limits*

$$\lim_{n\to\infty} \langle \psi_{\rho_n}, \widetilde{H}_p \, \psi_{\rho_n} \rangle \tag{4.87}$$

exist, where $\widetilde{H}_p$ is the fluctuation Hamiltonian of the extended mean-field model $H_{p,n}$ of H_n around some purification $|\psi\rangle\langle\psi|$ of ρ, cf. Eq. (4.78)*. On the other hand, if a sequence of true Bosonic ground states $\rho_{p,n}$ of $H_{p,n}$ has root-n fluctuations around a pure mean-field minimizer $|\psi\rangle\langle\psi|$ of $H_{p,\infty}$, then the sequence of reduced states $\mathrm{Tr}_{\mathcal{K}^{\otimes n}}(\rho_{p,n})$ is a sequence of true ground states of H_n, by Eq.* (4.64)*, and has root-n fluctuations around its mean-field minimizer $\mathrm{Tr}_{\mathcal{K}}(|\psi\rangle\langle\psi|)$ by Eq.* (4.83)*. Therefore, in order to answer the question whether there exists a sequence of true ground states of H_n that has root-n fluctuations around a minimizer of H_∞, cf. Rem. 4.2.4, it is sufficient to answer it in general for Bosonic systems.*

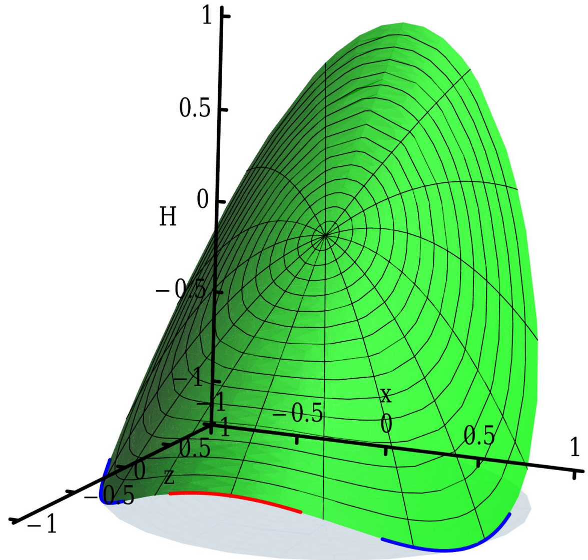

Figure 4.1.: Hamiltonian function $H = H_\infty(x,z)$ of the mean-field Ising model (4.89), where $y = 0$, $B = 1$ and $J = -1$. The minimizers in this parameter setting are $\rho^\pm$ (4.90), indicated by the blue lines along the boundary of H_∞. For $J \geq -\frac{B}{2}$, the minimizer is ρ_0, indicated by the red line along the boundary of H_∞.

4.5. Mean-field Ising model in transverse field

In this section, we perform the ground-state energy estimation for the mean-field Ising model, given by the Hamiltonian density $H_n = \operatorname{sym}_n H_2$ with

$$H_2 = B\sigma_z \otimes \mathbb{1} + J\sigma_x \otimes \sigma_x. \tag{4.88}$$

The related mean-field limiting function amounts to

$$H_\infty(\rho) = \rho^{\otimes 2}(H_2) = B \cdot z + J \cdot x^2, \tag{4.89}$$

where $\alpha = \rho(\sigma_\alpha)$ for $\alpha = x, y, z$ are the components of ρ in the Pauli basis. First, we identify the minimizers of the function, cf. Fig. 4.1. For $B > 0$, the minimizers amount to

$$\arg\min_\rho H_\infty(\rho) = \begin{cases} \rho_0 \cong (0,0,-1), & J \geq -\frac{B}{2} \\ \rho^\pm \cong \big((\pm\sin\phi, 0, \cos\phi)\big), & J \leq -\frac{B}{2}, \end{cases} \tag{4.90}$$

where $\phi = \arccos\left(\frac{B}{2J}\right)$.

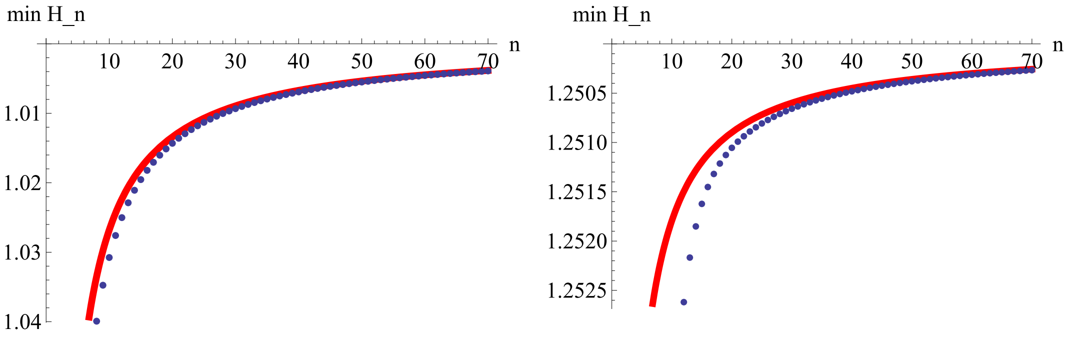

Figure 4.2.: Ground-state energy of H_n, for different values of n. Left: $B = 1$, $J = 1$ with mean-field minimizer ρ_0. Right: $B = 1$, $J = -1$ with mean-field minimizer $\rho^{\pm}$. Red lines: Functions (4.98) (left) and (4.110) (right). Blue dots: ground-state energy obtained by exact diagonalization.

Case $J \geq -\frac{B}{2}$

We begin with the case $J \geq -\frac{B}{2}$. We consider the computational basis $\{|0\rangle, |1\rangle\}$, such that $\rho_0 = |1\rangle\langle 1|$. The mean-field ground-state energy amounts to $H_\infty(\rho_0) = -B$ and the gradient and Hessian of H_∞ are given by

$$\begin{aligned} \mathrm{d}H_\infty(\rho_0) &= B \cdot \mathrm{d}z(\rho_0) + 2Jx \cdot \mathrm{d}x(\rho_0) = 2B\,|0\rangle\langle 0|\,, \\ \mathrm{d}_2 H_\infty(\rho_0) &= 2J \cdot \mathrm{d}x(\rho_0) \otimes \mathrm{d}x(\rho_0). \end{aligned} \tag{4.91}$$

Since $\rho_0 \cdot \mathrm{d}H_\infty(\rho_0) = \mathrm{d}H_\infty(\rho_0) \cdot \rho_0 = 0$, $\widehat{\mathrm{d}H_\infty}(\rho_0) = 0$, and

$$\begin{aligned} \widehat{\widehat{\mathrm{d}H_\infty}}(\rho_0) &= 2B\,\widehat{\widehat{|0\rangle\langle 0|}} \\ &= 2Ba^*a \\ &= B\left(Q^2 + P^2\right) - B\mathbb{1}, \end{aligned} \tag{4.92}$$

where $a = \widehat{|1\rangle\langle 0|}$ and $a^* = \widehat{|0\rangle\langle 1|}$ are the ladder operators of the fluctuation algebra and Q and P are the related canonical variables, defined by

$$Q = \frac{1}{\sqrt{2}}(a + a^*) \text{ and} \tag{4.93}$$

$$P = \frac{-i}{\sqrt{2}}(a - a^*). \tag{4.94}$$

With these, we also identify the fluctuators $\widehat{\sigma}_x = \sqrt{2}Q$ and $\widehat{\sigma}_y = -\sqrt{2}P$, which is in accordance with the commutator $\left[\widehat{\sigma}_x, \widehat{\sigma}_y\right] = -2i\mathbb{1}$. The fluctuator of the Hessian therefore amounts to

$$\begin{aligned} \widehat{\mathrm{d}_2 H_\infty}(\rho_0) &= 2J\left(\widehat{\sigma}_x \cdot \widehat{\sigma}_x - \mathbb{1}\right) \\ &= 4J \cdot Q^2 - 2J \cdot \mathbb{1}, \end{aligned} \tag{4.95}$$

where in the first line we used the fluctuator decomposition rule (3.15). Hence, the total fluctuation Hamiltonian amounts to

$$\begin{aligned}\widehat{H}(\rho_0) &= \widehat{\widehat{\mathrm{d}H_\infty}}(\rho_0) + \frac{1}{2}\widehat{\mathrm{d}_2 H_\infty}(\rho_0)\\ &= (B+2J)\,Q^2 + BP^2 - (B+J)\,\mathbb{1}\\ &= \sqrt{B\,(B+2J)}\cdot\left(Q'^2 + P'^2\right) - (B+J)\mathbb{1}.\end{aligned} \tag{4.96}$$

In the last line we performed a canonical transformation to $Q' = \alpha\cdot Q$ and $P' = P/\alpha$ with $\alpha = ((B+2J)/B)^{1/4}$, to obtain a harmonic oscillator in the standard form. Hence, its ground-state energy amounts to

$$\inf \widehat{H}(\rho_0) = \sqrt{B\,(B+2J)} - (B+J) \tag{4.97}$$

and the ground-state energy of the total system

$$\min H_n \le -B - \frac{1}{n}\left(B + J - \sqrt{B\,(B+2J)}\right). \tag{4.98}$$

Case $J \le -\frac{B}{2}$

In this case, the two mean-field minimizers amount to

$$\rho^\pm \cong \left(\pm\sin\phi,\, 0,\, \cos\phi\right), \tag{4.99}$$

with $\cos\phi = \frac{B}{2J}$. We will treat the fluctuations around both reference states in parallel and see that they lead to the same $1/n$ corrections. The mean-field ground-state energy amounts to $H_\infty(\rho^\pm) = J + \frac{B^2}{4J}$. It is convenient to rotate the minimizers into the σ_z-direction. This can be achieved by the rotation matrix

$$R = \begin{pmatrix}\cos\Theta & -\sin\Theta\\ \sin\Theta & \cos\Theta\end{pmatrix}, \tag{4.100}$$

with $\Theta = \mp\frac{\phi}{2}$, defining

$$\begin{aligned}\rho'^\pm &= R\rho R^T = |0\rangle\langle 0|\\ \sigma_x' &= R^T\sigma_x R = \cos\phi\cdot\sigma_x \mp \sin\phi\cdot\sigma_z\\ \sigma_z' &= \pm\sin\phi\cdot\sigma_x + \cos\phi\cdot\sigma_z.\end{aligned} \tag{4.101}$$

We switch to this rotated basis and omit the apostrophes for notational convenience. Hence, the reference state is $\rho^\pm \cong (0,0,1)$ in this new basis and the Hamiltonian function reads

$$H_\infty(\rho) = B\cdot(\cos\phi\cdot z \pm \sin\phi\cdot x) + J\cdot(\cos\phi\cdot x \mp \sin\phi\cdot z)^2. \tag{4.102}$$

The gradient and the Hessian in this basis amount to

$$\begin{aligned}\mathrm{d}H_\infty(\rho) = &\Big(B\cos\phi \mp 2J\sin\phi\cdot\big(\cos\phi\cdot x \mp \sin\phi\cdot z\big)\Big)\mathrm{d}z(\rho)\\ &+ \Big(\pm B\sin\phi + 2J\cos\phi\cdot\big(\cos\phi\cdot x \mp \sin\phi\cdot z\big)\Big)\mathrm{d}x(\rho)\end{aligned} \tag{4.103}$$

and

$$\begin{aligned} \mathrm{d}_2 H_\infty(\rho) &= 2J(\sin\phi)^2 \mathrm{d}z(\rho)^{\otimes 2} + 2J(\cos\phi)^2 \mathrm{d}x(\rho)^{\otimes 2} \\ &\quad \mp 2J\sin\phi\cos\phi \cdot \big(\mathrm{d}z(\rho)\otimes \mathrm{d}x(\rho) + \mathrm{d}x(\rho)\otimes \mathrm{d}z(\rho)\big). \end{aligned} \tag{4.104}$$

At the reference state $\rho^\pm \cong (0,0,1)$ the differentials amount to $\mathrm{d}x(0,0,1) = \sigma_x$ and $\mathrm{d}z(0,0,1) = \sigma_z - \mathbb{1} = -2\,|1\rangle\langle 1|$. We therefore obtain

$$\begin{aligned} \mathrm{d}H_\infty(\rho^\pm) &= -4J\,|1\rangle\langle 1| \text{ and} \\ \mathrm{d}_2 H_\infty(\rho^\pm) &= 8J(\sin\phi)^2 \cdot \big(|1\rangle\langle 1|\big)^{\otimes 2} + \frac{B^2}{2J}\cdot \sigma_x^{\otimes 2} \\ &\quad \pm 2B\sin\phi\big(\sigma_x \otimes |1\rangle\langle 1| + |1\rangle\langle 1| \otimes \sigma_x\big), \end{aligned} \tag{4.105}$$

where we substituted $\cos\phi = \frac{B}{2J}$ and $(\sin\phi)^2 = 1 - \frac{B^2}{4J^2}$. Hence, using the normal modes $a = \widehat{|0\rangle\langle 1|}$, $a^* = \widehat{|1\rangle\langle 0|}$ and the related canonical variables Q and P, we obtain

$$\begin{aligned} \widehat{\mathrm{d}H_\infty}(\rho^\pm) &= -4Ja^*a \\ &= -2J\left(Q^2 + P^2\right) + 2J\mathbb{1}, \end{aligned} \tag{4.106}$$

and

$$\begin{aligned} \widehat{\mathrm{d}_2 H_\infty}(\rho^\pm) &= \frac{B^2}{2J}\cdot\left(\widehat{\sigma}_x^2 - \mathbb{1}\right) \\ &= \frac{B^2}{J}Q^2 - \frac{B^2}{2J}\mathbb{1}, \end{aligned} \tag{4.107}$$

using $\widehat{\sigma}_x = \sqrt{2}Q$, and the fact that the fluctuators of $\big(|1\rangle\langle 1|\big)^{\otimes 2}$ and $\sigma_x \otimes |1\rangle\langle 1|$, resp. $|1\rangle\langle 1| \otimes \sigma_x$ vanish, due to $\rho^\pm \cdot |1\rangle\langle 1| = |1\rangle\langle 1| \cdot \rho^\pm = 0$. Hence, the fluctuation Hamiltonian amounts to

$$\begin{aligned} \widehat{H}(\rho^\pm) &= \widehat{\mathrm{d}H_\infty}(\rho^\pm) + \frac{1}{2}\widehat{\mathrm{d}_2 H_\infty}(\rho^\pm) \\ &= -2J\left(Q^2 + P^2\right) + \frac{B^2}{2J}Q^2 + \left(2J - \frac{B^2}{4J}\right)\mathbb{1} \\ &= \sqrt{4J^2 - B^2}\left(Q'^2 + P'^2\right) + \left(2J - \frac{B^2}{4J}\right)\mathbb{1}, \end{aligned} \tag{4.108}$$

where in the last line we performed a canonical transformation to $Q' = \beta\cdot Q$ and $P' = P/\beta$ with $\beta = (1 - \frac{B^2}{(2J)^2})^{1/4}$, to obtain a harmonic oscillator in the standard form. The ground-state energy of the fluctuation Hamiltonian therefore amounts to

$$\inf \widehat{H}(\rho^\pm) = \sqrt{4J^2 - B^2} + 2J - \frac{B^2}{4J}, \tag{4.109}$$

and the ground-state energy of the total system,

$$\min H_n \le J + \frac{B^2}{4J} + \frac{1}{n}\left(\sqrt{4J^2 - B^2} + 2J - \frac{B^2}{4J}\right), \quad J \le -\frac{B}{2}. \tag{4.110}$$

Comparison with exact diagonalization

We perform an exact diagonalization of the mean-field Ising model in the Bosonic sector. Using the angular momentum representation,

$$L_\alpha = \frac{n}{2}\,\mathrm{sym}_n\,\sigma_\alpha, \quad \alpha \in \{x,y,z\}, \tag{4.111}$$

we can write the Hamiltonian density in the following form

$$\begin{aligned} H_n &= B \cdot \mathrm{sym}_n\,\sigma_z + J \cdot \mathrm{sym}_n(\sigma_x \otimes \sigma_x) \\ &= \frac{2B}{n} L_z + J\left(\frac{n}{n-1}\big(\mathrm{sym}_n\,\sigma_x\big)^2 - \frac{1}{n-1}\mathbb{1}\right) \\ &= \frac{2B}{n} L_z + \frac{4J}{n(n-1)} L_x^2 - \frac{J}{n-1}\mathbb{1}. \end{aligned} \tag{4.112}$$

The obtained ground-state energies for two sets of parameter values and the related mean-field and fluctuation solutions (4.98), (4.110) are depicted in Fig. 4.2. We fit the exact data to a power series in orders of $1/n$ and extract the coefficients for the zeroth and first order. We find that they are in agreement with the theoretical values to a certain extent. The closer the parameter values B and J are to $B = -2J$, the less reliable convergence can be achieved. On the contrary, with parameter values far away from $B = -2J$ the results are in good agreement. For fitting the ground-state energies from 60 to 160 particles (with an increment of 10 particles), the analytical and fitted $1/n$-coefficients are in agreement for $(B,J) = (1,-1)$ up to the 6th significant digit and for $(B,J) = (1,1)$ up to the 8th. The change of the mean-field minimizer at the point $B = -2J$ is a quantum phase transition, due to the non-analyticity of the ground-state energy at this point [94]. It is understood, that at this point quantum fluctuations diverge. This is manifested by the fact, that the higher-order coefficients of the ground-state energy become very large, such that the $1/n$ correction (which is analytically computable at the transition point and is the same for both types of reference states, ρ_0 and $\rho^\pm$) cannot approximate the corrections to the mean-field ground-state energy well for any finite n.

4.5.1. Bosonic Ising model in transverse field

Since the mean-field minimizers of the mean-field Ising model are pure, we can also perform the fluctuations in the Bosonic formalism and obtain the same results. To show this, we use the notation from Section 4.3.3, i.e. the equations $D = \langle 1|\,\mathrm{d}f\,|1\rangle + \langle 10|\,\mathrm{d}_2 f\,|01\rangle$ (4.53) and $C = \langle 00|\,\mathrm{d}_2 f\,|11\rangle$ (4.54), in order to compute the frequency $\omega = \sqrt{D^2 - |C|^2}$ and the ground-state energy

$$E_0 = \frac{1}{2}\Big(\sqrt{D^2 - |C|^2} - D\Big). \tag{4.113}$$

Case $J \geq -\frac{B}{2}$

In this case, the minimizer is defined by $\rho_0 = |1\rangle\langle 1|$, hence we need to exchange the definition of $|0\rangle$ and $|1\rangle$ in D and C. Then, by Eq. (4.91), we obtain $D = 2(B+J)$ and $C = 2J$, such that $\omega = 2\sqrt{B(B+2J)}$ and $E_0 = \sqrt{B(B+2J)} - (B+J)$, reproducing (4.97).

Case $J \leq -\frac{B}{2}$

In this case, after transforming the minimizer to $\rho^+ = |0\rangle\langle 0|$, we obtain $D = -4J + \frac{B^2}{2J}$ and $C = \frac{B^2}{2J}$, such that $\omega = 2\sqrt{4J^2 - B^2}$ and $E_0 = \sqrt{4J^2 - B^2} + 2J - \frac{B^2}{4J}$, reproducing (4.109).

4.6. Bosonic systems and Bose-Einstein condensates

In recent years, the field of Bose-Einstein condensation has been an attractive research field [69, 85]. In particular, the experimental implementation [44] of the Bose-Hubbard model (BHM), which was originally invented as a toy model for Helium [37], with atoms confined in an optical lattice, has sparked renewed interest in the theoretical investigation of such systems [66]. The BHM describes a hard-core Bosonic lattice gas, with energy contributions for hopping among neighbouring sites (quantified by a parameter $-J$ with $|J| \geq 0$) and interaction (repulsion) of Bosons on each site (quantified by a parameter $U \geq 0$). Despite its simplicity, the BHM shows very interesting behaviour in the thermodynamic limit at low temperatures, in particular the quantum phase transition between Mott insulator and Bose-Einstein condensate (BEC).

The thermodynamic limit is defined by taking the particle number n and the volume V (or respectively the number of lattice sites d) to infinity, while leaving their ratio n/V (or n/d), constant. The definition of a BEC is, that in the limit the one-particle reduced density matrix of the ground state has one large eigenvalue, while all other eigenvalues vanish as $n \to \infty$, i.e. that it is (approximately) pure [69][4]. At zero temperature, the ground state is a BEC, if in the Hamiltonian the hopping-term is favoured over the on-site repulsion, i.e. $J \gg U$. If, on the other hand, the on-site repulsion dominates, then BEC is supressed in the ground state and the Mott-insulator phase, defined by an energy gap [69], occurs. Such a gap does not exist for BEC [69], hence the two phases exclude each other.

In this section, we treat the BHM as a strictly symmetric sequence by imposing a scaling on the on-site interaction term. We take the limit of infinitely many particles, $n \to \infty$, while leaving the number of lattice sites, d, constant. This limit is known

[4] In the literature concerning the Bose-Hubbard model, it is often spoken of superfluidity instead of BEC. Indeed, a BEC of mutually repulsive particles on a lattice will show superfluidity, in the sense that the one-particle wave function is being spread out over the whole lattice and the non-existence of a gap in the excitation spectrum, rendering the particles mobile w.r.t. the application of external forces [85]. In general, the relation between BEC and superfluidity is subtle, and in particular it is not known whether a universal definition of superfluidity exists [69]. In this section, we will treat the two notions as synonymous.

as the large-filling or mean-field limit. It may be primarily relevant for experimental implementations, e.g. in optical lattices, where the number of lattice sites is fixed. In this limit, the ground state is always a BEC, in the sense that the mean-field minimizer is by definition pure, cf. Section 4.3. We show that the fluctuation Hamiltonian around the minimizer is exactly the Bogoliubov Hamiltonian. The consequence is that the Bogoliubov method [15], which was originally invented as an approximation for the thermodynamic limit and has been criticized for not predicting the Mott phase, should be viewed as the first-order correction to the mean-field limit, which is a priori completely unrelated to the thermodynamic limit. Similar results were published earlier for the continuous case, i.e. Bose gases in a box with no lattice structure on it. It was shown for this case, that the Bogoliubov method gives the exact $1/n$-corrections to the ground-state energy [104, 67], complementing our result for the lattice case.

Our method does not address the thermodynamic limit, since the number of lattice sites is kept fixed. However, it would be interesting to see if our result can be extended in the sense that the fluctuation Hamiltonian is extrapolated for $d \to \infty$. In general, we do not assume that the limits $n \to \infty$ and $d \to \infty$ exchange, but in the parameter regime, in which BEC occurs, this may be the case. However, this step is beyond the scope of this thesis.

Furthermore, in Section 4.9 we will propose an extension of the fluctuation method to a class of approximately symmetric Hamiltonians. We will show that the BHM - without the artificial mean-field scaling - is a member this class. Hence, in principle it may be possible to obtain first-order corrections to the ground-state energy of that BHM. The obtained limit will still be a mean-field or large-filling limit, but due to the absence of the artificial scaling of the on-site interaction term the resulting properties may be substantially different.

4.6.1. A generic Bosonic lattice model as a mean-field model

Consider a lattice with d sites. A quantum particle in this lattice can be described by the Hilbert space $\mathcal{H} = \mathbb{C}^d$. An orthonormal basis of this space is given by $\left\{ |e_x\rangle \,\middle|\, x = 1, ..., d \right\}$, where the vector $|e_x\rangle$ corresponds to the particle being located at site x. Operators on the one-particle Hilbert space are spanned by the matrix elements $e_{xy} = |e_x\rangle \langle e_y|$.

A system of n Bosons in this lattice is described by the Hilbert space $\mathcal{H}_n = \mathrm{Sym}_n \, \mathcal{H}^{\otimes n}$, the Bosonic subspace of $\mathcal{H}^{\otimes n}$. Usually, Bosonic systems are described in Fock space $\mathfrak{F} = \mathbb{C} \oplus \mathcal{H} \oplus \mathcal{H}_2 \oplus ...$ using the Bosonic creation and annihilation operators c_x^*, c_x, which correspond to the creation/annihilation of a Boson at the lattice site x, for $x \in \{1, ..., d\}$.

A generic k-body Hamiltonian, which does not change particle number, can be written as

$$H = \sum_{x_1,...,x_k} \sum_{y_1,...,y_k} h(x_1, ..., x_k, y_1, ..., y_k) c_{x_1}^* c_{y_1} ... c_{x_k}^* c_{y_k}, \tag{4.114}$$

where the ordering of the creation/annihilation operators can be achieved using the commutation relations $[c_x, c_y^*] = \delta_{xy} \mathbb{1}$. Considering only the n-particle subspace of the Fock space $\mathfrak{F}$, it is possible to write the creation and annihilation operators in terms of angular momenta in the sense [111]

$$
\begin{aligned}
c_x^* c_y \restriction \mathcal{H}_n &= \sum_{i=1}^{n} \mathbb{1}^{\otimes i-1} \otimes |x\rangle \langle y| \otimes \mathbb{1}^{\otimes n-i} \\
&= n \cdot \mathrm{sym}_n \, e_{xy}.
\end{aligned}
\tag{4.115}
$$

Therefore, with the right scaling of $h(x_1, ..., x_k, y_1, ..., y_k)$ in n, the system amounts to a mean-field model.

4.6.2. The Bose-Hubbard model on a one-dimensional lattice

In the following, we consider the BHM on a one-dimensional lattice with d lattice sites and periodic boundary conditions (pp. 416, eq. 114.48 in [85]). By introducing the factor $1/(n-1)$ on the on-site interaction term, we make it a strictly symmetric mean-field model. We show that the related fluctuation Hamiltonian is exactly the well-known Bogoliubov Hamiltonian. Hence, we show that the Bogoliubov theory gives the $1/n$-corrections to the mean-field ground-state energy of the scaled BHM. A related result was derived before in [111], using assumptions not required by our method. Namely, in [111] Bose symmetry was enforced on the 2-particle level without justifying that this corresponds to Bose symmetry on the n-particle system as well. However, the mean-field minimizer of this modified model over the full one-particle state space was pure, such that Bose symmetry was automatically implemented, cf. Sect. 4.3. Furthermore, a complementary result has been known for infinite dimensional Bosons with weak interaction [104].

The Hamiltonian of the BHM in Fock space $\mathfrak{F}$ is given by

$$
H = \sum_{x=1}^{d} h_x c_x^* c_x - J \sum_{x=1}^{d} \left(c_{x+1}^* c_x + c_x^* c_{x+1} \right) + \frac{U}{2} \sum_{x=1}^{d} c_x^* c_x \left(c_x^* c_x - \mathbb{1} \right),
\tag{4.116}
$$

where c_x and c_x^* are particle annihilation and creation operators on the lattice site x. For convenience, we assume $h_x = 0$ for all x and $J \geq 0$ and $U \geq 0$. This allows for a simple computation of the mean-field minimizer.

We perform a Fourier transformation into momentum space, in which the mean-field minimizer will be a basis state, instead of a uniform superposition over all basis states. We introduce the momentum-annihilation operators

$$
c_p = \frac{1}{\sqrt{d}} \sum_{x=1}^{d} e^{ipx} c_x,
\tag{4.117}
$$

where

$$
p = \frac{\pi}{d} \cdot \begin{cases} (0, 2, 4, ..., 2(d-1)) - d & , d \text{ even} \\ (0, 2, 4, ..., 2(d-1)) - (d-1) & , d \text{ odd}. \end{cases}
\tag{4.118}
$$

The Hamiltonian then amounts to

$$
H = \sum_{p}^{d} h_p c_p^* c_p + \frac{U}{2d} \sum_{r,s,p,q}^{d} \delta_{r+s,p+q} c_r^* c_s^* c_p c_q,
\tag{4.119}
$$

where $h_p = -2J\cos(p)$. Since the Hamiltonian conserves the particle number, we can restrict it to some fixed particle number n and obtain the following identity

$$\begin{aligned}(c_p^* c_q) \restriction \mathcal{H}_n &= \sum_{i=1}^{n} \mathbb{1}^{\otimes i-1} \otimes |p\rangle\langle q| \otimes \mathbb{1}^{\otimes n-i} \\ &= n \cdot \mathrm{sym}_n(e_{pq}),\end{aligned} \tag{4.120}$$

where $e_{pq} = |p\rangle\langle q|$ with $|p\rangle$ and $|q\rangle$ being basis vectors of the one-particle Hilbert space $\mathcal{H}$ in the momentum basis. Thus,

$$H \restriction \mathcal{H}_n =: n \cdot H_n^{(n)} = n \cdot \mathrm{sym}_n\, H_2^{(n)}, \tag{4.121}$$

with

$$H_2^{(n)} = \sum_p^d \frac{h_p}{2}(e_{pp} \otimes \mathbb{1} + \mathbb{1} \otimes e_{pp}) + \frac{g^{(n)}}{2d} \sum_{r,s,p,q}^{d} \delta_{r+s,p+q} e_{rp} \otimes e_{sq}. \tag{4.122}$$

Note that $H_n^{(n)}$ is not a strictly or approximately symmetric sequence, because the coefficient $g^{(n)} := U \cdot (n-1)$ scales with n. In order to circumvent this issue, we introduce the mean-field scaling by replacing $g^{(n)} \mapsto g = g^{(N_0)}$, $H_2^{(n)} \mapsto H_2 = H_2^{(N_0)}$ and therefore $H_n^{(n)} \mapsto H_n = H_n^{(N_0)}$ for all n, with some fixed N_0. That is, H_n is the mean-field model related to the N_0-particle system. In the following, we derive the mean-field limit and the fluctuation Hamiltonian around the mean-field minimizer for this model. The mean-field limiting function of H_n at a point $\rho \in \mathcal{S}(\mathcal{H})$ amounts to

$$H_\infty(\rho) = \sum_p^d h_p \rho_{pp} + \frac{g}{2d} \sum_{r,s,p,q}^{d} \delta_{r+s,p+q} \rho_{rp} \cdot \rho_{sq}, \tag{4.123}$$

with $\rho_{pq} = \rho(e_{pq})$. The gradient and the Hessian are given by

$$\mathrm{d}H_\infty(\rho) = \sum_p^d h_p \mathrm{d}e_{pp}(\rho) + \frac{g}{d} \sum_{r,s,p,q}^{d} \delta_{r+s,p+q} \rho_{rp} \cdot \mathrm{d}e_{sq}(\rho) \text{ and} \tag{4.124}$$

$$\mathrm{d}_2 H_\infty(\rho) = \frac{g}{d} \sum_{r,s,p,q}^{d} \delta_{r+s,p+q} \mathrm{d}e_{rp}(\rho) \otimes \mathrm{d}e_{sq}(\rho), \tag{4.125}$$

where $\mathrm{d}e_{pq}(\rho) = e_{pq} - \rho_{pq}\mathbb{1}$.

In the following, we show that the discrete time-dependent Gross-Pitaevskii equation [85] is equivalent to the Hartree equation $\dot{\rho} = -i[\rho, \mathrm{d}H_\infty(\rho)]$ in this model. We switch to the location-basis $\{|x\rangle, x = 1, ..., d\}$, where the mean-field limiting function amounts to

$$H_\infty(\rho) = \sum_{x=1}^{d} \Big(h_x \rho_{xx} + \frac{U}{2}\rho_{xx}^2 - J(\rho_{x+1,x} + \rho_{x,x+1}) \Big), \tag{4.126}$$

with $\rho_{xy} = \rho(e_{xy})$. The gradient therefore amounts to

$$\mathrm{d}H_\infty(\rho) = \sum_{x=1}^{d} \Big(\big(h_x + U\rho_{xx}\big)\mathrm{d}e_{xx}(\rho) - J\big(\mathrm{d}e_{x+1,x}(\rho) + \mathrm{d}e_{x,x+1}(\rho)\big) \Big), \tag{4.127}$$

with $\mathrm{d}e_{xy}(\rho) = e_{xy} - \rho_{xy}\mathbb{1}$. If we consider a pure state $\rho = |\psi\rangle\langle\psi|$ with $|\psi\rangle = \sum_{x=1}^{d}\psi_x|x\rangle$, then the Hartree equation, $\dot{\rho} = -i[\rho, \mathrm{d}H_\infty(\rho)]$, leads to

$$i\dot{\psi}_x = \left(h_x + U|\psi_x|^2\right)\psi_x - J\left(\overline{\psi}_{x+1}\psi_x + \overline{\psi}_x\psi_{x+1}\right) \quad \forall x, \tag{4.128}$$

which is just the discrete version of the time-dependent Gross-Pitaevski equation [85].

We switch back to the momentum basis $\{|p\rangle\}$ and continue with the ground-state energy estimation. The state $\rho = |p\rangle\langle p|$ with $p = 0$ is a minimizer of H_∞ (4.123) on the pure submanifold $\mathcal{S}_{\mathrm{pure}}(\mathcal{H})$. The value of H_∞ at this point, i.e. the mean-field ground-state energy, amounts to

$$H_\infty\big(|0\rangle\langle 0|\big) = \frac{g}{2d} - 2J. \tag{4.129}$$

In the following, we omit the ρ-dependence on all differentials, i.e., we write $\mathrm{d}f := \mathrm{d}f\big(|0\rangle\langle 0|\big)$ for all f. At this point, the gradient amounts to

$$\mathrm{d}H_\infty = \sum_p h_p \mathrm{d}e_{pp}, \tag{4.130}$$

since

$$\sum_{r,s,p,q}^{d}\delta_{r+s,p+q}\rho_{rp}\cdot\mathrm{d}e_{sq} = \sum_p \mathrm{d}e_{pp} = \sum_p e_{pp} - \mathbb{1} = 0. \tag{4.131}$$

The Hessian amounts to

$$\mathrm{d}_2H_\infty = \frac{g}{d}\sum_{r,s,p,q}^{d}\delta_{r+s,p+q}\mathrm{d}e_{rp}\otimes\mathrm{d}e_{sq}. \tag{4.132}$$

Clearly, the minimum conditions (4.22) and (4.24) are fulfilled: $\mathrm{d}H_\infty|0\rangle = 0$ and

$$\begin{aligned}&\langle q0|\,\mathrm{d}_2H_\infty\,|0q\rangle + \langle q|\,\mathrm{d}H_\infty\,|q\rangle - |\langle qq|\,\mathrm{d}_2H_\infty\,|00\rangle|\\ =&\frac{g}{d} + h_q - h_0\\ =&\frac{U}{d}(N_0 - 1) + 2J(1-\cos(q)) \geq 0 \quad \forall\,|q\rangle\perp|0\rangle,\ \forall J,U\geq 0.\end{aligned} \tag{4.133}$$

Next, we construct the fluctuation Hamiltonian $\widehat{H}$. By Prop. 3.6.1, the normal modes of the fluctuation algebra at $\rho = |0\rangle\langle 0|$ are given by $a_p = \widehat{e_{0p}}$ and $a_p^* = \widehat{e_{p0}}$, for $p \neq 0$. Moreover, $\widehat{e_{pq}} = 0$ and $\widehat{\widehat{e_{pq}}} = a_p^*a_q$, for $p,q\neq 0$. Especially, we have

$$\widehat{\widehat{e_{pp}}} = \begin{cases} a_p^*a_p & ,\ p\neq 0\\ -\sum_{p'\neq 0}a_{p'}^*a_{p'} & ,\ p = 0\end{cases}. \tag{4.134}$$

Finally, note that $\widehat{e_{pq}} = \widehat{\mathrm{d}e_{pq}}$ by construction, cf. Eq. (2.33). Hence, the fluctuators of the gradient and Hessian amount to

$$\widehat{\widehat{\mathrm{d}H_\infty}} = \sum_{p\neq 0}(h_p - h_0)a_p^*a_p \tag{4.135}$$

and

$$\begin{aligned}
\widehat{\mathrm{d}_2 H_\infty} &= \frac{g}{d} \sum_{r,s,p,q} \delta_{r+s,p+q} \operatorname{Fluct}_\infty\big(\mathrm{d}e_{rp} \otimes \mathrm{d}e_{sq}\big) \\
&= \frac{g}{d} \sum_{r,s,p,q} \delta_{r+s,p+q} \big(\widehat{e_{rp}} \cdot \widehat{e_{sq}} - \rho(\mathrm{d}e_{rp} \cdot \mathrm{d}e_{sq})\mathbb{1}\big) \\
&= \frac{g}{d} \sum_{r,s,p,q} \delta_{r+s,p+q} \big((\delta_{r0} a_p + \delta_{p0} a_r^*) \cdot (\delta_{s0} a_q + \delta_{q0} a_s^*) - \delta_{r0}\delta_{q0}\delta_{ps}\mathbb{1} + \delta_{r0}\delta_{p0}\delta_{s0}\delta_{q0}\mathbb{1}\big) \\
&= \frac{g}{d} \sum_{p \neq 0} \big(a_p^* a_p + a_p a_p^* + a_p a_{-p} + a_p^* a_{-p}^*\big) - \frac{g(d-1)}{d}\mathbb{1} \\
&= \frac{g}{d} \sum_{p \neq 0} \big(2a_p^* a_p + a_p a_{-p} + a_p^* a_{-p}^*\big),
\end{aligned} \tag{4.136}$$

where in the last line we used $(d-1)\mathbb{1} = \sum_{p\neq 0}[a_p, a_p^*]$. Hence, the fluctuation Hamiltonian amounts to

$$\begin{aligned}
\widehat{H} &= \widehat{\widehat{\mathrm{d}H_\infty}} + \frac{1}{2}\widehat{\mathrm{d}_2 H_\infty} \\
&= \sum_{p\neq 0} \left(h_p - h_0 + \frac{g}{d}\right) a_p^* a_p + \sum_{p\neq 0} \frac{g}{2d} \left(a_p a_{-p} + a_p^* a_{-p}^*\right) \\
&= \frac{1}{2} \sum_{p\neq 0} \Big(\alpha_p\big(a_p^* a_p + a_{-p}^* a_{-p}\big) + \beta\big(a_p a_{-p} + a_p^* a_{-p}^*\big)\Big),
\end{aligned} \tag{4.137}$$

where $\alpha_p = h_p - h_0 + \frac{g}{d}$ and $\beta = \frac{g}{d}$. Also, in the last line we used the fact that in the sum for each value of p, the value $-p$ is contained as well, and that $\alpha_p = \alpha_{-p}$ for all p.

The fluctuation Hamiltonian $\widehat{H}$ is exactly the well-known Bogoliubov Hamiltonian [85]. Therefore, the rather heuristic Bogoliubov approximation coincides with the $1/n$-corrections for the mean-field limit. It is important to note, that the ladder operators a_p, a_p^* of the fluctuation algebra have nothing to do with the particle annihilation/creation operators c_p, c_p^* of the original system. In particular, the fluctuation algebra contains one mode less. This fact seems to be not contained or emphasized in the heuristic Bogoliubov approach (Cf. pp. 226ff in [85]).

Furthermore, in Section 5.4, we show that the time evolution of the fluctuations around the mean-field minimizer of the BHM is generated exactly by the Bogoliubov Hamiltonian, provided that Conj. 5.3.2 holds.

4.6.3. Note on higher-dimensional lattices

The fluctuation method can be performed on any lattice or interaction type. The generalization to higher-dimensional lattices is straightforward. However, in general it can be difficult to define the fluctuation Hamiltonian. The obstacle is finding the mean-field minimizer, i.e. the minimum of the mean-field Hamiltonian H_∞, which is a non-linear function over d complex parameters.

4.7. Inner bound for the finite de Finetti problem

Consider a permutation invariant state $\rho_n \in \mathcal{A}_n$ with $\mathcal{A} = \mathcal{B}(\mathcal{H})$ and $\dim \mathcal{H} = d$. Its k-particle reduced state, $\rho_n^{(k)}$, is called n-exchangable. The finite de Finetti theorem [23, 63, 17] tells how close this state is to the set of de Finetti states. More precisely, there exists a probability measure μ on $\mathcal{S}(\mathcal{A})$ and a related de Finetti state

$$\rho_{\mu,k} = \int_{\mathcal{S}(\mathcal{A})} \mu(\mathrm{d}\rho)\, \rho^{\otimes k}, \tag{4.138}$$

such that

$$\left\| \rho_{\mu,k} - \rho_n^{(k)} \right\|_1 \leq \frac{2kd^2}{n}, \tag{4.139}$$

where $\|.\|_1$ denotes the trace norm [23], cf. Sect. 2.5. Since this bound holds for all n-exchangable states, we can also express it with the supremum over them, that is

$$\sup_{\rho_n} \inf_{\mu} \left\| \rho_{\mu,k} - \rho_n^{(k)} \right\|_1 \leq \frac{2kd^2}{n}. \tag{4.140}$$

In this sense, the finite de Finetti bound limits the maximal distance of the n-exchangable states to the set of de Finetti states. In this section, we will derive an inner bound, namely the minimal distance, that the farthest n-exchangable state is away from the set of de Finetti states. To do so, we show that the left-hand side (4.140) can be expressed as a mean-field ground-state problem. That is,

$$\begin{aligned}
\sup_{\rho_n} \inf_{\mu} \left\| \rho_{\mu,k} - \rho_n^{(k)} \right\|_1 &= \sup_{\rho_n} \inf_{\mu} \sup_{H_k} \left(\rho_{\mu,k}(H_k) - \rho_n^{(k)}(H_k) \right) \\
&= \sup_{H_k} \sup_{\rho_n} \inf_{\mu} \left(\rho_{\mu,k}(H_k) - \rho_n^{(k)}(H_k) \right) \\
&= \sup_{H_k} \left(\inf_{\sigma} \sigma^{\otimes k}(H_k) - \inf_{\rho_n} \rho_n(\mathrm{sym}_n(H_k)) \right) \\
&= \sup_{H_k} \left(\inf H_\infty - \inf H_n \right).
\end{aligned} \tag{4.141}$$

In the first line, we just inserted the definition of the trace norm. It suffices to take the supremum over hermitian H_k, with $\|H_k\| \leq 1$, since the density operators are hermitian as well. Also, it is not necessary to consider an absolute value, since with H_k also $-H_k$ is included in the supremum. The second line follows from an application of the minmax theorem [53], while in the third line the supremum over ρ_n and the infimum over μ relate to the two different terms independently. In the fourth line, we defined the function $H_\infty(\rho) = \rho^{\otimes k}(H_k)$, which is the mean-field limit of the Hamiltonian density $H_n = \mathrm{sym}_n H_k$. The infima $\inf H_\infty$ and $\inf H_n$ denote the respective ground-state energies. Hence, estimating the left-hand side of (4.141) is equivalent to estimating the $1/n$-corrections to the ground-state energy of H_n. By Thm. 4.2.2 we therefore obtain the inequality

$$\sup_{\rho_n} \inf_{\mu} \left\| \rho_{\mu,k} - \rho_n^{(k)} \right\|_1 \geq -\frac{1}{n} \inf_{H_k} \inf_{\rho_0} \left(\inf \widehat{H}(\rho_0) \right) \tag{4.142}$$

for n large enough, where $\widehat{H}(\rho_0) = \widehat{\widehat{\mathrm{d}H_\infty}}(\rho_0) + \frac{1}{2}\widehat{\mathrm{d}_2 H_\infty}(\rho_0)$ is the fluctuation Hamiltonian of H_∞ at ρ_0 and $\inf \widehat{H}(\rho_0)$ denotes its ground-state energy. The infima in Eq. (4.142) go over all minimizers ρ_0 of $H_\infty = \mathrm{sym}_\infty H_k$ and all hermitian H_k with $\|H_k\| \leq 1$.

4.8. Relation to the Holstein-Primakoff transformation

The Holstein-Primakoff representation is a widely used tool in many-body physics [10]. Considering a Lie algebra generated by the spin operators S_α for $\alpha \in \{x, y, z\}$, with a total spin S, the representation amounts to

$$\begin{aligned} S_z &= S - a^* a, \\ S_+ &= \sqrt{2S - a^* a} \cdot a \quad \text{and} \\ S_- &= a^* \cdot \sqrt{2S - a^* a}, \end{aligned} \tag{4.143}$$

where $S_\pm = S_x \pm i S_y$ and a and a^* are Bosonic annihilation and creation operators. When states with spin much lower than S are considered, then the square roots can be approximated by

$$\begin{aligned} S_x &= \sqrt{\frac{S}{2}}\,(a + a^*) \ \text{ and} \\ S_y &= -i\sqrt{\frac{S}{2}}\,(a - a^*)\,, \end{aligned} \tag{4.144}$$

simplifying computations significantly. One method, that uses the Holstein-Primakoff approximation is spin-wave theory [10], which emerges when considering a system of many spins and assuming that each spin is large, such that the approximation (4.144) holds. The spin waves are then states of the system consisting of n Bosonic modes, which is constructed by applying (4.143) to each spin. This method is however not related to the mean-field theory presented in this thesis and will therefore not be considered further.

On the other hand, the Holstein-Primakoff approximation is also used for permutation invariant (or *long-range*) models, for example the Lipkin-Meshkov-Glick model [70]. In the following, we consider systems consisting of spin-$\frac{1}{2}$ particles, to keep the notation simple. A generalization to higher one-particle dimensions is nevertheless straightforward. We define angular momentum operators by

$$S_\alpha = \frac{n}{2}\,\mathrm{sym}_n\,\sigma_\alpha, \quad \alpha \in \{x, y, z\}. \tag{4.145}$$

In terms of the Schur-Weyl decomposition, cf. Eq. (2.54), these operators can be written as

$$S_\alpha = \bigoplus_j \mathbb{1}_{\mathcal{H}_j} \otimes S_\alpha^{(j)}, \tag{4.146}$$

where the index j takes values in $\{0, 1, ..., \frac{n}{2}\}$ for n even and $\{\frac{1}{2}, \frac{3}{2}, ..., \frac{n}{2}\}$ for n odd. Each value of j represents a Young diagram Y in the sense that the number of boxes in its second row amounts to j for n even and $j - \frac{1}{2}$ for n odd. For each j, $S_\alpha^{(j)}$ is a generator of the Lie algebra with total angular momentum j and one can find a basis consisting of $S_z^{(j)}$-eigenvectors $\left|\psi_m^{(j)}\right\rangle$, with the relation

$$S_z^{(j)} \left|\psi_m^{(j)}\right\rangle = (j - m) \left|\psi_m^{(j)}\right\rangle . \tag{4.147}$$

It is now straightforward to apply the Holstein-Primakoff transformation (4.143) to each angular momentum operator $S_\alpha^{(j)}$. However, independent of n, (4.146) contains some spins $S_\alpha^{(j)}$ with a small j, such that the approximation (4.144) does not hold. But on the other hand, the model is often restricted to Bosonic particles, i.e. symmetric vectors in $\mathcal{H}^{\otimes n}$, such that only the $\left(j = \frac{n}{2}\right)$–sector is considered. Clearly, in this sector the large-j limit corresponds to the large-n limit, such that (4.144) holds if n is large enough.

We show the analogy between the fluctuation method and the Holstein-Primakoff approximation for the mean-field Ising model. We applied the fluctuation method in Section 4.5. The Hamiltonian density of the mean-field Ising model is given by

$$\begin{aligned} nH_n &= -nB \operatorname{sym}_n \sigma_z + nJ \operatorname{sym}_n \sigma_x \otimes \sigma_x \\ &= -2BS_z + \frac{4J}{n-1} S_x^2 - \frac{nJ}{n-1} \mathbb{1}, \end{aligned} \tag{4.148}$$

where we choose the coupling to the magnetic field to be $-B$ with $B > 0$. If $2J \geq -B$, then the mean-field minimizer amounts to $\rho_0 = |0\rangle \langle 0|$ with $\rho_0(\sigma_z) = 1$. It is therefore polarized in the z-direction, such that we can apply the Holstein-Primakoff approximation (4.144) to the spin operators and obtain

$$\begin{aligned} nH_n &= -n \cdot B\mathbb{1} + 2Ba^* a + J(a + a^*)^2 - J\mathbb{1} + O\left(\frac{1}{n}\right) \\ &= -n \cdot B\mathbb{1} - B\left(Q^2 + P^2 - \mathbb{1}\right) + 2JQ^2 - J\mathbb{1} + O\left(\frac{1}{n}\right) \\ &= -n \cdot B\mathbb{1} + \sqrt{B(B+2J)}\left(Q'^2 + P'^2\right) - (J+B)\mathbb{1} + O\left(\frac{1}{n}\right), \end{aligned} \tag{4.149}$$

where, as in Section 4.5, we introduced the position and momentum operators Q and P, cf. Eq. (4.93), and transformed them to Q', P', to obtain the standard form, cf. Eq. (4.96). In the third line, the first term is just the mean-field ground-state energy and the other non-vanishing terms are exactly the fluctuation Hamiltonian (4.96).

In [33], it was shown that the Holstein-Primakoff approximation does not give the optimal $1/n$-corrections to the ground-state energy of the Lipkin-Meshkov-Glick model. However, this does not contradict our remark on the optimality of the fluctuations method, cf. Rem. 4.2.4, because this model is approximately but not strictly symmetric (cf. Section 4.9), while the fluctuation method presented in this thesis only applies to the latter class of mean-field models.

4.9. Ground-state estimation for approximately symmetric Hamiltonians

Above, we performed the ground-state estimation only for strictly symmetric Hamiltonian densities. However, there also exist physically interesting approximately symmetric models. For example, for the Lipkin-Meshkov-Glick model [70, 33], the Hamiltonian density can be written as

$$\begin{aligned} H_n &= -\frac{\lambda}{2n^2}\sum_{i\neq j}\left(\sigma_x^{(i)}\sigma_x^{(j)} + \gamma\sigma_y^{(i)}\sigma_y^{(j)}\right) - \frac{h}{n}\sum_i \sigma_z^{(i)} \\ &= -\frac{\lambda}{2n}\frac{n-1}{n}\operatorname{sym}_n\left(\sigma_x\otimes\sigma_x + \gamma\sigma_y\otimes\sigma_y\right) - h\operatorname{sym}_n\sigma_z \\ &= \operatorname{sym}_n A_2 + \frac{1}{n}\operatorname{sym}_n B_2, \end{aligned} \tag{4.150}$$

where $A_2 = -h\sigma_z\otimes\mathbb{1} - \frac{\lambda}{2}\left(\sigma_x\otimes\sigma_x + \gamma\sigma_y\otimes\sigma_y\right)$ and $B_2 = -\frac{\lambda}{2}\left(\sigma_x\otimes\sigma_x + \gamma\sigma_y\otimes\sigma_y\right)$. Clearly, this is an approximately symmetric sequence.

In the following, we consider a subset of approximately symmetric Hamiltonian densities, defined by

$$H_n = \operatorname{sym}_n A_k + \frac{1}{n^\epsilon}\operatorname{sym}_n B_l, \tag{4.151}$$

with $\epsilon > 0$. Note that this class does not include all approximately symmetric sequences, but it suffices to outline the difficulties that occur when trying to implement the fluctuation method. The main problem is the choice of the reference state for the fluctuation algebra. If some reference state ρ is chosen, then it is possible to implement the Taylor expansion (2.41) in the following way

$$H_n = \sum_{r=0}^{k}\frac{1}{r!n^{\frac{r}{2}}}\widetilde{\mathrm{d}_r A_\infty}(\rho) + \frac{1}{n^\epsilon}\left(\sum_{s=0}^{l}\frac{1}{s!n^{\frac{s}{2}}}\widetilde{\mathrm{d}_s B_\infty}(\rho)\right). \tag{4.152}$$

where $A_\infty = \operatorname{sym}_\infty A_k$ and $B_\infty = \operatorname{sym}_\infty B_l$. Note that since the mean-field limiting function is just $H_\infty = A_\infty$, the Taylor expansion of H_∞ would neglect the B–terms. Furthermore, the B–terms lead to corrections to the mean-field limit of order $n^{-\epsilon}$, which are more significant then n^{-1} for $\epsilon < 1$. Hence, the naive implementation of the fluctuation method to H_∞ would not give the right corrections to the mean-field ground-state energy.

A possible way to estimate the ground-state energy for finite n is to obtain the reference state by minimizing H_n over product states, which is different from minimizing the mean-field limiting function H_∞, i.e.

$$\rho^{(n)} = \arg\min_\rho \rho^{\otimes n}(H_n) \neq \arg\min_\rho H_\infty(\rho). \tag{4.153}$$

Then we define the fluctuation algebra $\mathcal{F}_{\rho^{(n)}}$ around $\rho^{(n)}$ and estimate the asymptotic behaviour of expectation values of (4.152) up to some order with sequences of states with root-n fluctuations around $\rho^{(n)}$. If it is possible to obtain a convenient parametrization of the reference states $\rho^{(n)}$ and the related fluctuation Hamiltonians $\widetilde{H}^{(n)}$, then it may be possible to obtain a suitable asymptotic expansion of (4.152) with suitable sequences ρ_n and to minimize over such sequences accordingly.

Finally, we show that it is possible to consider the Bose-Hubbard model as an approximately symmetric sequence, without relying on the artificial mean-field scaling, cf. Sect. 4.6.2. Considering Eq. (4.122), since the total energy scales with n^2 in leading order, we may just define the Hamiltonian as

$$H \upharpoonright \mathcal{H}_n := n^2 K_n \tag{4.154}$$

with the approximately symmetric sequence

$$K_n = \mathrm{sym}_n\, A_2 + \frac{1}{n}\,\mathrm{sym}_n\, B_2, \tag{4.155}$$

where

$$A_2 = \frac{U}{2d} \sum_{r,s,p,q} \delta_{r+s,p+q}\, e_{rp} \otimes e_{sq} \quad \text{and} \tag{4.156}$$

$$B_2 = \sum_p \frac{h_p}{2} (e_{pp} \otimes \mathbb{1} + \mathbb{1} \otimes e_{pp}) - \frac{U}{2d} \sum_{r,s,p,q} \delta_{r+s,p+q} e_{rp} \otimes e_{sq}. \tag{4.157}$$

5. Time evolution of mean-field fluctuations

5.1. Overview

In this chapter, we consider the dynamical aspects of mean-field fluctuators. In their seminal paper, Hepp and Lieb proved that the fluctuation property is preserved for a class of Hamiltonian dynamics [52]. That is, if a sequence ρ_n has root-n fluctuations around ρ, then the time-evolved sequence $\rho_{t,n} = \rho_n \circ T_{t,n}$ has root-n fluctuations around $\rho_t = \mathcal{F}_t \rho$, where $T_{t,n}$ is the Heisenberg time evolution and $\mathcal{F}_t$ is the related mean-field limiting flow, cf. Section 2.3.

The theorem was stated for the case of the Hamiltonian density being of the form $H_n = F(\operatorname{sym}_n H^{(1)}, \operatorname{sym}_n H^{(2)}, ..., \operatorname{sym}_n H^{(3)})$, where F is a polynomial with n-independent coefficients and $H^{(i)} \in \mathcal{A}$ for all i. We were not able to lift the proof to general strictly symmetric Hamiltonian densities $H_n = \operatorname{sym}_n H_k$, but we show that the time derivative for finite particle number n supports this conjecture.

In Section 5.2, we derive the time evolution of differential forms and show that it is implemented by the Jacobian $J_t(\rho)$ of the mean-field limiting Hamiltonian flow $\mathcal{F}_t$. Moreover, we introduce coordinates for the manifold $\mathcal{S}(\mathcal{A})$, which enables us to derive the differential equations for the Jacobian $J_t(\rho)$ and the differential form $\mathrm{d}(f \circ \mathcal{F}_t)(\rho)$ for differentiable $f \in \mathcal{C}(\mathcal{S}(\mathcal{A}))$.

In Section 5.3, we state the theorem of Hepp and Lieb [52] and propose a related time evolution for fluctuators of mean-field systems with strictly symmetric Hamiltonian densities $H_n = \operatorname{sym}_n H_k$. We compute the time derivative of fluctuators for finite n, supporting our conjecture. We show that the derivative amounts to the generator of the Jacobian time evolution plus a term of order $1/\sqrt{n}$. In this project, we were not able to bound the $O(1/\sqrt{n})$-terms sufficiently, such that the time derivative could be integrated to finite times in the limit, which is why we have to leave the statement of the time evolution of fluctuators with strictly symmetric Hamiltonian densities as a conjecture.

Finally, in Section 5.4, we consider the case in which the reference state ρ of the fluctuation algebra is a minimizer of the mean-field limiting Hamiltonian H_∞. We show that in this case the time evolution of fluctuators is implemented by a Hamiltonian and that, provided the above conjecture holds, this Hamiltonian is exactly the fluctuation Hamiltonian $\widehat{H}(\rho)$, which we introduced in Chapter 4 to obtain the $1/n$-corrections to the mean-field ground-state energy.

A similar result has been found for mean-field systems consisting of infinite-dimensional Bosons [9]. In this case, the tools from differential geometry could not be applied. However, it was shown there, that the variance of the limiting Gaussian distribution is determined by a time-dependent Bogoliubov transformation describing the dynamics of initial coherent states in a Fock-space representation of the system. Furthermore, it was shown that the time evolution of fluctuations around Hartree states is generated by a corresponding Bogoliubov Hamiltonian [68], thus complementing our results for the case of infinite-dimensional Bosons.

5.2. Time evolution of differential forms

In this section, we consider the time evolution of differential forms $\mathrm{d}f_t(\rho)$, where $f_t = f \circ \mathcal{F}_t$ for $f \in \mathcal{C}(\mathcal{S}(\mathcal{A}))$ and $\mathcal{F}_t$ being a Hamiltonian flow on $\mathcal{S}(\mathcal{A})$, defined by a twice differentiable function $H_\infty \in \mathcal{C}(\mathcal{S}(\mathcal{A}))$, cf. Sect. 2.3. We will introduce the Jacobian

$$J_t(\rho)\colon T^*_{\rho_t}\mathcal{S}(\mathcal{A}) \to T^*_\rho\mathcal{S}(\mathcal{A}) \tag{5.1}$$

of the flow $\mathcal{F}_t$, which implements the time evolution of differential forms by

$$\mathrm{d}f_t(\rho) = J_t(\rho)\big(\mathrm{d}f(\rho_t)\big), \tag{5.2}$$

where $\rho_t = \mathcal{F}_t\rho$. The basic structure of $J_t(\rho)$ was presented in [31] for general mean-field dynamical semigroups. Here, we make the structure precise for the mean-field limit of dynamics generated by $nH_n \in \mathcal{A}_n$ with a strictly symmetric Hamiltonian density $H_n = \mathrm{sym}_n H_k$. In Section 5.2.1, we introduce coordinates for the manifold $\mathcal{S}(\mathcal{A})$, which we use in Section 5.2.2 to define the Jacobian and derive its structure.

5.2.1. Coordinate description

In this section, we introduce coordinates for the manifold $\mathcal{S}(\mathcal{A})$ and the tangent and co-tangent spaces. This will simplify the computation of Jacobian dynamics.

Consider the one-particle operator algebra $\mathcal{A} = \mathcal{B}(\mathcal{H})$ with $\dim\mathcal{H} = d$ as a Hilbert space with the Hilbert-Schmidt scalar product $\langle A, B\rangle = \mathrm{Tr}(A^*B)$. Define an orthogonal basis of hermitian operators $\{e^i,\ i = 0,\dots,d^2-1\}$ in $\mathcal{A}$, where $e^0 = \mathbb{1}$ and all others are traceless. The e^i are commonly known as the generalized Gell-Mann or generalized Pauli matrices [11]. The dual basis in $\mathcal{A}^*$ is given by the set $\{e_i,\ i = 0,\dots,d^2-1\}$, defined by $\langle e_i, e^j\rangle = \mathrm{Tr}(e_i^* e^j) = \delta_i^j$, such that the e_i are hermitian and traceless as well[1].

Let $\kappa = d^2 - 1$. A density operator $\rho \in \mathcal{S}(\mathcal{A})$ can be parametrized by

$$\rho = \frac{1}{d}\Big(\mathbb{1} + \sum_{i=1}^{\kappa} x^i e_i\Big), \tag{5.3}$$

where $\{x^1,\dots,x^\kappa\} \in \mathbb{R}^\kappa$. It is important to note that not every vector $\{x^1,\dots,x^\kappa\}$ defines a density matrix this way. Indeed, positivity and unit-trace of ρ must be ensured. Nevertheless, it is clear that the set of vectors defining the state space $\mathcal{S}(\mathcal{A})$ is a convex subset of $\mathbb{R}^\kappa$. Hence, the tangent and cotangent spaces are isomorphic to the vector space $\mathbb{R}^\kappa$ at each $\rho \in \mathcal{S}(\mathcal{A})$.

[1] As before, despite the isomorphy $\mathcal{A} \cong \mathcal{A}^*$, we keep the formal distinction between $\mathcal{A}$ and $\mathcal{A}^*$, since it enables us to distinguish between the tangent and cotangent spaces $T_\rho\mathcal{S}(\mathcal{A})$ and $T^*_\rho\mathcal{S}(\mathcal{A})$, which is relevant due to the choice of representatives of the latter in $\mathcal{A}$.

For the tangent space $T_\rho\mathcal{S}(\mathcal{A}) \cong \mathbb{R}^\kappa$ at $\rho \in \mathcal{S}(\mathcal{A})$, we define the basis

$$\left\{ \frac{\partial}{\partial x^i}\Big|_\rho \;\Big|\; i = 1, \dots, \kappa \right\}. \tag{5.4}$$

The dual basis, of the cotangent space $T^*_\rho\mathcal{S}(\mathcal{A})$, will be denoted by $\{\mathrm{d}x^i(\rho);\ i = 1, \dots, \kappa\}$. We fix the choice of representatives on $\mathcal{A}$ again by $\rho(\mathrm{d}x^i(\rho)) = 0$, such that we can identify

$$\mathrm{d}x^i(\rho) = e^i - \rho(e^i)\mathbb{1} \in \mathcal{A}. \tag{5.5}$$

It follows that due to the bilinear form between $\mathcal{A}^*$ and $\mathcal{A}$ (given by the Hilbert-Schmidt scalar product), we can identify $\frac{\partial}{\partial x^i}\Big|_\rho = e_i \in \mathcal{A}^*$, independent of ρ. In other words, the bilinear map between $T_\rho\mathcal{S}(\mathcal{A})$ and $T^*_\rho\mathcal{S}(\mathcal{A})$ can be written as

$$\left\langle \frac{\partial}{\partial x^i}\Big|_\rho \;\Big|\; \mathrm{d}x^j(\rho) \right\rangle = \langle e_i, e^j \rangle = \mathrm{Tr}(e_i\, e^j) = \delta^j_i. \tag{5.6}$$

Note that $e_i = e_i^*$ and that the choice of representative of $\mathrm{d}x^j(\rho)$ is irrelevant, because $\mathrm{Tr}(e_i \cdot \mathbb{1}) = 0$ for all $1 \le i \le \kappa$.

5.2.2. Time evolution of differential forms

In this section, we derive the time evolution of differential forms $\mathrm{d}f_t(\rho) \in T^*_\rho\mathcal{S}(\mathcal{A})$. Let $H_\infty \in \mathcal{C}(\mathcal{S}(\mathcal{A}))$ be a twice differentiable function and consider the related generator L of the nonlinear flow $\mathcal{F}_t$, given by

$$L\rho = -i[\mathrm{d}H_\infty(\rho), \rho]. \tag{5.7}$$

In the following, we write $\rho_t = \mathcal{F}_t\rho$ for the time evolved state. On the function $f \in \mathcal{C}(\mathcal{S}(\mathcal{A}))$, the mean-field time evolution is given by

$$f_t(\rho) = T_{t,\infty}f(\rho) = f(\rho_t) = f \circ \mathcal{F}_t(\rho). \tag{5.8}$$

The time evolution of the related differential form, $\mathrm{d}f_t(\rho)$, is determined by the Jacobian $J_t(\rho)$ of the flow $\mathcal{F}_t$ by

$$J_t(\rho)\big(\mathrm{d}f(\rho_t)\big) = \mathrm{d}(f \circ \mathcal{F}_t)(\rho). \tag{5.9}$$

In coordinates, this equation amounts to

$$J_t(\rho)\left(\sum_j \frac{\partial f}{\partial x^j}\Big|_{\rho_t} \mathrm{d}x^j(\rho_t) \right) = \sum_{ij} \frac{\partial \mathcal{F}_t^j}{\partial x^i}\Big|_\rho \frac{\partial f}{\partial x^j}\Big|_{\rho_t} \mathrm{d}x^i(\rho). \tag{5.10}$$

Hence, $J_t(\rho)\colon T^*_{\rho_t}\mathcal{S}(\mathcal{A}) \to T^*_\rho\mathcal{S}(\mathcal{A})$ is a linear map with the coefficients

$$J_t(\rho)^j_i = \frac{\partial \mathcal{F}_t^j}{\partial x^i}\Big|_\rho. \tag{5.11}$$

In the following, we introduce a bra-ket notation, derived from (5.6), to consider $J_t(\rho)$ as a linear map. That is, we write

$$J_t(\rho) = \sum_{i,j} J_t(\rho)_i^j \left|\mathrm{d}x^i(\rho)\right\rangle \left\langle \frac{\partial}{\partial x^j}\Big|_{\rho_t}\right| \tag{5.12}$$

Then, considering $a \in T^*_{\rho_t}\mathcal{S}(\mathcal{A})$ as a vector, i.e. $a = \sum_{k=1}^{\kappa} a_k \left|\mathrm{d}x^k(\rho_t)\right\rangle$, the application of $J_t(\rho)$ amounts to

$$\begin{aligned} J_t(\rho)(a) &= \sum_{i,j,k} J_t(\rho)_i^j a_k \left|\mathrm{d}x^i(\rho)\right\rangle \left\langle \frac{\partial}{\partial x^j}\Big|_{\rho_t}\right|\left.\mathrm{d}x^k(\rho_t)\right\rangle \\ &= \sum_{i,j} J_t(\rho)_i^j a_j \left|\mathrm{d}x^i(\rho)\right\rangle \\ &= \sum_{i,j} J_t(\rho)_i^j a_j \, \mathrm{d}x^i(\rho). \end{aligned} \tag{5.13}$$

In the following, we derive the time derivative of $\mathrm{d}f_t(\rho)$. By the product rule, we get

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{d}f_t(\rho) = \dot{J}_t(\rho)\big(\mathrm{d}f(\rho_t)\big) + J_t(\rho)\left(\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{d}f(\rho_t)\right). \tag{5.14}$$

We start with computing $\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{d}f(\rho_t)$, i.e.

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\mathrm{d}f(\rho_t) &= \sum_i \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial f}{\partial x^i}\Big|_{\rho_t} \cdot \mathrm{d}x^i(\rho_t)\right) \\ &= \sum_{ij} \frac{\mathrm{d}\mathcal{F}_t^j}{\mathrm{d}t}\Big|_{\rho} \cdot \frac{\partial^2 f}{\partial x^j \partial x^i}\Big|_{\rho_t} \mathrm{d}x^i(\rho_t) + \sum_i \frac{\partial f}{\partial x^i}\Big|_{\rho_t} \cdot \frac{\mathrm{d}}{\mathrm{d}t}\mathrm{d}x^i(\rho_t) \\ &= \sum_{ij} (L\rho_t)^j \cdot \frac{\partial^2 f}{\partial x^j \partial x^i}\Big|_{\rho_t} \mathrm{d}x^i(\rho_t) - \sum_i \frac{\partial f}{\partial x^i}\Big|_{\rho_t} \cdot (L\rho_t)^i \mathbb{1} \\ &= \sum_{ijk} \frac{\partial^2 f}{\partial x^i \partial x^j}\Big|_{\rho_t} \cdot (L\rho_t)^k \left\langle \frac{\partial}{\partial x^k}\Big|_{\rho_t}\right|\left.\mathrm{d}x^j(\rho_t)\right\rangle \cdot \mathrm{d}x^i(\rho_t) - \langle L\rho_t, \mathrm{d}f(\rho_t)\rangle \mathbb{1} \\ &= \mathrm{Tr}_2\big((\mathbb{1} \otimes L\rho_t) \cdot \mathrm{d}_2 f(\rho_t)\big) - \mathrm{Tr}\big(L\rho_t \cdot \mathrm{d}f(\rho_t)\big)\mathbb{1} \\ &= \mathrm{Tr}_2\Big(\big(\mathbb{1} \otimes \rho_t\big) \cdot i\big[\mathbb{1} \otimes \mathrm{d}H_\infty(\rho_t),\, \mathrm{d}_2 f(\rho_t)\big]\Big) - \mathrm{Tr}\Big(\rho_t \cdot i\big[\mathrm{d}H_\infty(\rho_t),\, \mathrm{d}f(\rho_t)\big]\Big)\mathbb{1} \\ &= \mathrm{id} \otimes \rho_t\big(i[\mathbb{1} \otimes \mathrm{d}H_\infty(\rho_t),\, d_2 f(\rho_t)]\big) - \{H_\infty, f\}(\rho_t)\mathbb{1}. \end{aligned} \tag{5.15}$$

In the second line of (5.15), we applied the chain rule of derivatives. In the third line, we identified $\frac{\mathrm{d}\mathcal{F}_t^j}{\mathrm{d}t}\Big|_{\rho} = (L\rho_t)^j$ and

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{d}x^i(\rho_t) = \frac{\mathrm{d}}{\mathrm{d}t}\big(e^i - (\rho_t)^i \mathbb{1}\big) = -(L\rho_t)^i \mathbb{1}. \tag{5.16}$$

In the fourth line of (5.15) we included the Kronecker symbol δ^j_k and used Eq.(5.6), and in the fifth line we introduced the Hessian of f, which can be written as

$$\mathrm{d}_2 f(\rho_t) = \sum_{i,j} \frac{\partial^2 f}{\partial x^i \partial x^j}\Big|_{\rho_t} \mathrm{d}x^i(\rho_t) \otimes \mathrm{d}x^j(\rho_t). \tag{5.17}$$

Finally, we used the definition of $L\rho_t$ (5.7) and our notation $\rho(.)$ for expectation values with $\rho \in \mathcal{S}(\mathcal{A})$, and $\mathrm{id}(A) = A$ for $A \in \mathcal{A}$.

If considering a general μ-dependent state ρ_μ with $\mu \in \mathbb{R}$, then (5.15) can be generalized to

$$\frac{\mathrm{d}}{\mathrm{d}\mu} \mathrm{d}f(\rho_\mu) = \mathrm{Tr}_2\Big((\mathbb{1} \otimes \rho'_\mu) \cdot \mathrm{d}_2 f(\rho_\mu)\Big) - \mathrm{Tr}\Big(\rho'_\mu \cdot \mathrm{d}f(\rho_\mu)\Big)\mathbb{1}, \tag{5.18}$$

where $\rho'_\mu = \frac{\mathrm{d}}{\mathrm{d}\mu}\rho_\mu$.

Next, we compute $\dot{J}_t(\rho)$. The time derivative of the (j,i)-th component amounts to

$$\begin{aligned} \dot{J}_t(\rho)^j_i &= \frac{\mathrm{d}}{\mathrm{d}t} \frac{\partial \mathcal{F}^j_t}{\partial x^i}\Big|_\rho \\ &= \frac{\partial}{\partial t} \frac{\partial \mathcal{F}^j_t}{\partial x^i}\Big|_\rho \\ &= \frac{\partial}{\partial x^i} (L\mathcal{F}_t)^j\Big|_\rho \\ &= \sum_{k,l} \frac{\partial}{\partial x^i} \left(\frac{\partial H_\infty}{\partial x^k}\Big|_{\rho_t} \cdot (\rho_t)^l \right)\Big|_\rho \cdot \Big\langle -i[\mathrm{d}x^k(\rho_t),\, e^l] \Big| \, \mathrm{d}x^j(\rho_t) \Big\rangle, \end{aligned} \tag{5.19}$$

where in the last line we used the fact that the jth component of $\dot{\rho}_t = L\mathcal{F}_t\rho$ (cf. Eq. (5.7)) can be written as

$$(L\mathcal{F}_t\rho)^j = \Big\langle -i[\mathrm{d}H_\infty(\rho_t),\, \rho_t] \Big| \, \mathrm{d}x^j(\rho_t) \Big\rangle \tag{5.20}$$

and then used the basis-decomposition of $\mathrm{d}H_\infty(\rho_t)$ and ρ_t. The derivative in the last line of (5.19) amounts to

$$\begin{aligned} \frac{\partial}{\partial x^i} \left(\frac{\partial H_\infty}{\partial x^k}\Big|_{\rho_t} \cdot (\rho_t)^l \right)\Big|_\rho &= \sum_m \frac{\partial \mathcal{F}^m_t}{\partial x^i}\Big|_\rho \cdot \frac{\partial^2 H_\infty}{\partial x^m \partial x^k}\Big|_{\rho_t} \cdot (\rho_t)^l + \frac{\partial H_\infty}{\partial x^k}\Big|_{\rho_t} \cdot \frac{\partial \mathcal{F}^l_t}{\partial x^i}\Big|_\rho \\ &= \sum_m \Big(J_t(\rho)^m_i \cdot \mathrm{d}_2 H_\infty(\rho_t)_{m,k} \cdot (\rho_t)^l + \big(J_t(\rho)\big)^l_i \cdot \mathrm{d}H_\infty(\rho_t)_k \Big). \end{aligned} \tag{5.21}$$

We therefore obtain for all $a \in T^*_{\rho_t}\mathcal{S}(\mathcal{A})$

$$\dot{J}_t(\rho)(a) = J_t(\rho)\Big(\mathrm{id} \otimes \rho_t\Big(i\big[\mathrm{d}_2 H_\infty(\rho_t),\, \mathbb{1} \otimes a\big]\Big) + i\big[\mathrm{d}H_\infty(\rho_t),\, a)\big]\Big). \tag{5.22}$$

Moreover, we can write the differential equation for $J_t(\rho)$ as

$$\dot{J}_t(\rho) = J_t(\rho)\mathrm{d}L(\rho_t), \tag{5.23}$$

where $\mathrm{d}L(\rho_t)\colon T^*_{\rho_t}\mathcal{S}(\mathcal{A}) \to T^*_{\rho_t}\mathcal{S}(\mathcal{A})$ is the derivative of the generator of $\mathcal{F}_t$. Hence, the time derivative of the differential of a function $f_t = f \circ \mathcal{F}_t$ amounts to

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{d}f_t(\rho) = \quad & J_t(\rho)\Big(\mathrm{id}\otimes\rho_t\big(i\big[\mathrm{d}_2H_\infty(\rho_t),\, \mathbb{1}\otimes\mathrm{d}f(\rho_t)\big] + i\big[\mathbb{1}\otimes\mathrm{d}H_\infty(\rho_t),\, \mathrm{d}_2f(\rho_t)\big]\big)\Big)\\ & + J_t(\rho)\Big(i\big[\mathrm{d}H_\infty(\rho_t),\, \mathrm{d}f(\rho_t)\big] - \{H_\infty, f\}(\rho_t)\mathbb{1}\Big).\end{aligned} \tag{5.24}$$

Since we can write $\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{d}f_t(\rho) = \frac{\mathrm{d}}{\mathrm{d}\epsilon}\mathrm{d}f_{t+\epsilon}(\rho)|_{\epsilon=0}$ by the chain rule of derivatives, we can also write

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{d}f_t(\rho) = \quad & \mathrm{id}\otimes\rho\big(i\big[\mathrm{d}_2H_\infty(\rho),\, \mathbb{1}\otimes\mathrm{d}f_t(\rho)\big] + i\big[\mathbb{1}\otimes\mathrm{d}H_\infty(\rho),\, \mathrm{d}_2f_t(\rho)\big]\big)\\ & + i\big[\mathrm{d}H_\infty(\rho),\, \mathrm{d}f_t(\rho)\big] - \{H_\infty, f_t\}(\rho)\mathbb{1},\end{aligned} \tag{5.25}$$

since $J_0(\rho) = \mathrm{id}$. Furthermore, it is possible to show that the time derivative can be written as

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{d}f_t(\rho) = \mathrm{d}\{H_\infty,\, f_t\}(\rho), \tag{5.26}$$

i.e. as the gradient of the Poisson bracket $\{H_\infty,\, f_t\}$ at ρ. Indeed, if we compute $\sigma\big(\mathrm{d}\{H_\infty,\, g\}(\rho)\big)$ for some $\sigma \in \mathcal{S}(\mathcal{A})$ and $g \in \mathcal{C}(\mathcal{S}(\mathcal{A}))$, then using Def. 2.4.1 and Eq. (5.18) with $\rho_\mu = \rho + \mu(\sigma - \rho)$, we obtain

$$\begin{aligned}\sigma\big(\mathrm{d}\{H_\infty,\, g\}(\rho)\big) &= \frac{\mathrm{d}}{\mathrm{d}\mu}\{H_\infty,\, g\}(\rho_\mu)\Big|_{\mu=0}\\ &= \frac{\mathrm{d}}{\mathrm{d}\mu}\,\mathrm{Tr}\big(\rho_\mu\cdot i[\mathrm{d}H_\infty(\rho_\mu),\, \mathrm{d}g(\rho_\mu)]\big)\Big|_{\mu=0}\\ &= \mathrm{Tr}\big(\rho'_\mu\cdot i[\mathrm{d}H_\infty(\rho_\mu),\, \mathrm{d}g(\rho_\mu)]\big)\Big|_{\mu=0}\\ &\quad + \mathrm{Tr}\Big(\rho\cdot i\big([\mathrm{Tr}_2(\mathbb{1}\otimes\sigma\cdot\mathrm{d}_2H_\infty(\rho)),\, \mathrm{d}g(\rho)] + [\mathrm{d}H_\infty(\rho),\, \mathrm{Tr}_2(\mathbb{1}\otimes\sigma\cdot\mathrm{d}_2g(\rho))]\big)\Big)\\ &= \sigma\big(i[\mathrm{d}H_\infty(\rho),\, \mathrm{d}g(\rho)] - \rho(i[\mathrm{d}H_\infty(\rho),\, \mathrm{d}g(\rho)])\mathbb{1}\big)\\ &\quad + \mathrm{Tr}\Big((\rho\otimes\sigma)\cdot i\big([\mathrm{d}_2H_\infty(\rho),\, \mathrm{d}g(\rho)\otimes\mathbb{1}] + [\mathrm{d}H_\infty(\rho)\otimes\mathbb{1},\, \mathrm{d}_2g(\rho)]\big)\Big)\\ &= \sigma\Big(\mathrm{id}\otimes\rho\big(i\big[\mathrm{d}_2H_\infty(\rho),\, \mathbb{1}\otimes\mathrm{d}g(\rho)\big] + i\big[\mathbb{1}\otimes\mathrm{d}H_\infty(\rho),\, \mathrm{d}_2g(\rho)\big]\big)\\ &\qquad + i\big[\mathrm{d}H_\infty(\rho),\, \mathrm{d}g(\rho)\big] - \{H_\infty, g\}(\rho)\mathbb{1}\Big).\end{aligned} \tag{5.27}$$

Hence, by setting $g = f_t$, we obtain Eq. (5.25).

5.3. General fluctuation dynamics

In this section, we restate the theorem for fluctuation dynamics from [52] and provide a translation to our notation and setting. Most importantly, the class of Hamiltonian densities considered in [52] is given by $H_n = F(\mathrm{sym}_n H^{(1)}, \mathrm{sym}_n H^{(2)}, ..., \mathrm{sym}_n H^{(k)})$, where F is a polynomial with n-independent coefficients and $H^{(i)} \in \mathcal{A}$ for all i. Clearly, Hamiltonian densities of this type are approximately symmetric sequences and the related limiting functions are polynomials of finite degree, hence span the same dense subset of $\mathcal{C}(\mathcal{S}(\mathcal{A}))$ as the strictly symmetric sequences $H_n = \mathrm{sym}_n H_k$, with $H_k \in \mathcal{A}_k$. However, for finite n, they differ from strictly symmetric sequences by additional terms with factors of orders of $1/n$.

Furthermore, in [52] a (fixed) state ω on the inductive-limit algebra $\mathcal{A}^\infty = \overline{\bigcup_n \mathcal{A}^{\otimes n}}$ is considered. There, ω is called pure classical, if there exists a $\rho \in \mathcal{S}(\mathcal{A})$, such that every n-particle reduced state of ω amounts to $\rho^{\otimes n}$. In other words, by Størmer's de Finetti theorem [109], the pure classical states are the permutation invariant states on $\mathcal{A}^\infty$, that correspond to point measures on the manifold $\mathcal{S}(\mathcal{A})$.

Moreover, in [52] ω is said to have normal fluctuations, if for all products of fluctuators

$$\widetilde{A_i} = \sqrt{n}(\mathrm{sym}_n A_i - \rho(A_i)\mathbb{1}_n), \tag{5.28}$$

with $A_i \in \mathcal{A}$ and $\rho \in \mathcal{S}(\mathcal{A})$ defining the reduced states of ω, the limits

$$\lim_{n\to\infty} \omega\big(\widetilde{A_1} \cdot ... \cdot \widetilde{A_k}\big) = \big\langle \Omega_\omega, \widehat{A_1} \cdot ... \cdot \widehat{A_k}\, \Omega_\omega \big\rangle \tag{5.29}$$

exist. Clearly, their definition of fluctuations is equivalent to the one used in this thesis, cf. Def. 3.5.1, exept[2] for the fact that it is stated for the state ω on the inductive-limit space $\mathcal{A}^\infty$. Hence, Ω_ω is a vector on the fluctuation Hilbert space $\mathcal{H}_\rho$. Furthermore, a differential equation for the mean-field time evolution $\rho \mapsto \rho_t = \mathcal{F}_t \rho$ is given in [52], which is equal to the Hartree equation used in this thesis, cf. Eq. (2.46).

In [52], the time evolution of fluctuators was stated as follows.

Theorem 5.3.1 ([52]). *Consider a Hamiltonian density of the form*

$$H_n = F(\mathrm{sym}_n H^{(1)}, \mathrm{sym}_n H^{(2)}, ..., \mathrm{sym}_n H^{(k)}), \tag{5.30}$$

where F is a polynomial with n-independent coefficients and $H^{(i)} \in \mathcal{A}$ for all i. Consider the related Heisenberg time-evolution $T_{t,n}$ for finite n and $T_{t,\infty}$ for the mean-field limit, cf. Sect. 2.3. Furthermore, consider a pure classical state ω on $\mathcal{A}^\infty$, which has normal fluctuations and its reduced states being defined by $\rho \in \mathcal{S}(\mathcal{A})$. Then, for every product of time-evolved fluctuators

$$\widetilde{A_i(t)} := \sqrt{n}\big(T_{t,n}\, \mathrm{sym}_n A_i - \rho(T_{t,\infty} A_i)\mathbb{1}\big), \tag{5.31}$$

with $A_i \in \mathcal{A}$, the limits

$$\lim_{n\to\infty} \omega\big(\widetilde{A_1(t)} \cdot ... \cdot \widetilde{A_k(t)}\big) = \Big\langle \Omega_\omega, \widehat{A_1(t)} \cdot ... \cdot \widehat{A_k(t)}\, \Omega_\omega \Big\rangle \tag{5.32}$$

exist, where the $\widehat{A_i(t)}$ are solutions of the linear variational equation around the Hartree equation in [52] with the related initial condition ρ.

[2] Furthermore, their precise definition of fluctuators amounts to $\widetilde{A_i} = \sqrt{n}(\mathrm{sym}_n A_i - \gamma_i \mathbb{1})$, with some suitable $\gamma_i \in \mathbb{C}$. But the relation $\gamma_i = \rho(A_i)$ is evident.

In the following, we translate the theorem to our notation and state that the fluctuation evolution is given by the Jacobian time evolution of differentials. It is important to note that Thm. 5.3.1 applies to Hamiltonian densities of the type (5.30). Although the proof in [52] allows for the impression that it can be easily lifted to strictly symmetric Hamiltonian densities $H_n = \mathrm{sym}_n H_k$ with $H_k \in \mathcal{A}_k$, we were not able to prove it with different methods. We will comment on it more precisely at the end of this section. A straightforward translation of Thm. 5.3.1 can be phrased as follows

Conjecture 5.3.2. *Consider $\rho \in \mathcal{S}(\mathcal{A})$ and $H_n = \mathrm{sym}_n H_k$ with $H_k \in \mathcal{A}_k$ for some $k \in \mathbb{N}$. Note, that the sequence $\rho^{\otimes n}$ has root-n fluctuations around ρ. Then the sequence $\rho_{t,n} = \rho^{\otimes n} \circ T_{t,n}$ has root-n fluctuations around $\rho_t = \mathcal{F}_t \rho$ for all $t \geq 0$, where $T_{t,n}$ is the Heisenberg time evolution generated by H_n and $\mathcal{F}_t$ the related mean-field limiting flow on $\mathcal{S}(\mathcal{A})$, cf. Sect. 2.3. Moreover, the limiting expectation value of fluctuators $\widetilde{\mathrm{d}f(\rho_t)}, \widetilde{\mathrm{d}g(\rho_t)}\ldots$, for $f, g \in \mathcal{C}(\mathcal{S}(\mathcal{A}))$ amounts to*

$$\begin{aligned} &\lim_{n\to\infty} \rho_{t,n}\Big(\widetilde{\mathrm{d}f(\rho_t)} \cdot \widetilde{\mathrm{d}g(\rho_t)} \cdot \ldots\Big) = \Big\langle \Omega_t,\, \widetilde{\mathrm{d}f(\rho_t)} \cdot \widetilde{\mathrm{d}g(\rho_t)} \cdot \ldots \Omega_t \Big\rangle \\ &= \lim_{n\to\infty} \rho^{\otimes n}\Big(\widetilde{\mathrm{d}f_t(\rho)} \cdot \widetilde{\mathrm{d}g_t(\rho)} \cdot \ldots\Big) = \Big\langle \Omega,\, \widetilde{\mathrm{d}f_t(\rho)} \cdot \widetilde{\mathrm{d}g_t(\rho)} \cdot \ldots \Omega \Big\rangle, \end{aligned} \tag{5.33}$$

where $\mathrm{d}f_t(\rho) = J_t(\rho)\mathrm{d}f(\rho_t)$, and $\Omega \in \mathcal{H}_\rho$ and $\Omega_t \in \mathcal{H}_{\rho_t}$ are the limiting vectors for $\rho^{\otimes n}$ and $\rho_{t,n}$, respectively.

In the following, we compute the time derivative of fluctuators for finite n and show that it supports the conjecture. Indeed, the time derivative of an expectation value with fluctuators amounts to

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\rho_{t,n}\Big(\widetilde{\mathrm{d}f(\rho_t)} \cdot \widetilde{\mathrm{d}g(\rho_t)} \cdot \ldots\Big) &= \rho_{t,n} \circ G_n\Big(\widetilde{\mathrm{d}f(\rho_t)} \cdot \widetilde{\mathrm{d}g(\rho_t)} \cdot \ldots\Big) \\ &\quad + \rho_{t,n}\Big(\frac{\mathrm{d}}{\mathrm{d}t}\Big(\widetilde{\mathrm{d}f(\rho_t)} \cdot \widetilde{\mathrm{d}g(\rho_t)} \cdot \ldots\Big)\Big) \\ &= \rho_{t,n}\Big(\Big(i[nH_n,\, \widetilde{\mathrm{d}f(\rho_t)}] + \frac{\mathrm{d}}{\mathrm{d}t}\widetilde{\mathrm{d}f(\rho_t)}\Big) \cdot \widetilde{\mathrm{d}g(\rho_t)} \cdot \ldots\Big) \\ &\quad + \rho_{t,n}\Big(\widetilde{\mathrm{d}f(\rho_t)} \cdot \Big(i[nH_n,\, \widetilde{\mathrm{d}g(\rho_t)}] + \frac{\mathrm{d}}{\mathrm{d}t}\widetilde{\mathrm{d}g(\rho_t)}\Big) \cdot \ldots\Big) + \ldots, \end{aligned} \tag{5.34}$$

where $G_n(.) = i[nH_n, .]$ is the generator of the time evolution $T_{t,n}$.

Lemma 5.3.3. *Using the notation of this section, the time derivative of a fluctuator in (5.34) amounts to*

$$i[nH_n,\, \widetilde{\mathrm{d}f(\rho_t)}] + \frac{\mathrm{d}}{\mathrm{d}t}\widetilde{\mathrm{d}f(\rho_t)} = \mathrm{Fluct}\Big(\mathrm{d}\{H_\infty, f\}(\rho_t)\Big) + O\left(\frac{1}{\sqrt{n}}\right), \tag{5.35}$$

where the vanishing order, $O\left(1/\sqrt{n}\right)$, is understood in expectation in sequences ρ_n with root-n fluctuations around ρ_t.

Proof. We start with the commutator $i[nH_n, \widetilde{\mathrm{d}f(\rho_t)}]$. Using the Taylor expansion (2.41) and the product rule (2.7), it amounts to

$$\begin{aligned} i[nH_n, \widetilde{\mathrm{d}f(\rho_t)}] &= \sum_{r=1}^{k} \frac{1}{r!} in\sqrt{n}\big[\mathrm{sym}_n\, \mathrm{d}_r H_\infty(\rho_t),\, \mathrm{sym}_n\, \mathrm{d}f(\rho_t)\big] \\ &= \sum_{r=1}^{k} \frac{1}{(r-1)!}\sqrt{n}\,\mathrm{sym}_n\Big(i[\mathrm{d}_r H_\infty(\rho_t),\, \mathbb{1}^{\otimes(r-1)} \otimes \mathrm{d}f(\rho_t)]\Big). \end{aligned} \tag{5.36}$$

The time derivative of $\widetilde{\mathrm{d}f(\rho_t)}$, on the other hand, is given by Eq. (5.15) and amounts to

$$\frac{\mathrm{d}}{\mathrm{d}t}\widetilde{\mathrm{d}f(\rho_t)} = \sqrt{n}\,\mathrm{sym}_n\Big(\mathrm{id} \otimes \rho_t\big(i[\mathbb{1} \otimes \mathrm{d}H_\infty(\rho_t),\, d_2 f(\rho_t)]\big) - \{H_\infty, f\}(\rho_t)\mathbb{1}\Big). \tag{5.37}$$

Hence,

$$\begin{aligned} & i[nH_n, \widetilde{\mathrm{d}f(\rho_t)}] + \frac{\mathrm{d}}{\mathrm{d}t}\widetilde{\mathrm{d}f(\rho_t)} \\ =& \sqrt{n}\,\mathrm{sym}_n\Big(\mathrm{id} \otimes \rho_t\big(i[\mathbb{1} \otimes \mathrm{d}H_\infty(\rho_t),\, d_2 f(\rho_t)]\big) + i[\mathrm{d}H_\infty(\rho_t),\, \mathrm{d}f(\rho_t)] - \{H_\infty, f\}(\rho_t)\mathbb{1}\Big) \\ &+ \sum_{r=2}^{k} \frac{\sqrt{n}}{(r-1)!}\,\mathrm{sym}_n\big(i[\mathrm{d}_r H_\infty(\rho_t),\, \mathbb{1}^{\otimes(r-1)} \otimes \mathrm{d}f(\rho_t)]\big). \end{aligned} \tag{5.38}$$

What remains to be shown, is that the terms in the sum can be written as fluctuators, and that only the $(r = 2)$ - term remains in the limit and provides the remaining term for the definition of $\mathrm{Fluct}\big(\mathrm{d}\{H_\infty, f\}(\rho_t)\big)$. Indeed, by expanding $\mathrm{id} = \mathrm{id} \pm \mathcal{P}$, with the projector $\mathcal{P}(A) = \rho_t(A)\mathbb{1}$, $\forall A \in \mathcal{A}$, we obtain

$$\begin{aligned} & \frac{\sqrt{n}}{(r-1)!}\,\mathrm{sym}_n\big(i[\mathrm{d}_r H_\infty(\rho_t),\, \mathbb{1}^{\otimes(r-1)} \otimes \mathrm{d}f(\rho_t)]\big) \\ =& \frac{\sqrt{n}}{(r-1)!}\,\mathrm{sym}_n\Big((\mathrm{id} - \mathcal{P} + \mathcal{P})^{\otimes r}\big(i[\mathrm{d}_r H_\infty(\rho_t),\, \mathbb{1}^{\otimes(r-1)} \otimes \mathrm{d}f(\rho_t)]\big)\Big) \\ =& \frac{\sqrt{n}}{(r-1)!}\,\mathrm{sym}_n\Big((\mathrm{id} - \mathcal{P})^{\otimes r}\big(i[\mathrm{d}_r H_\infty(\rho_t),\, \mathbb{1}^{\otimes(r-1)} \otimes \mathrm{d}f(\rho_t)]\big)\Big) \\ &+ \frac{\sqrt{n}}{(r-1)!}\,\mathrm{sym}_n\Big((\mathrm{id} - \mathcal{P})^{\otimes(r-1)} \otimes \mathcal{P}\big(i[\mathrm{d}_r H_\infty(\rho_t),\, \mathbb{1}^{\otimes(r-1)} \otimes \mathrm{d}f(\rho_t)]\big)\Big) \\ =& \frac{1}{(r-1)! \cdot n^{(r-1)/2}} \cdot \mathrm{Fluct}\Big(i[\mathrm{d}_r H_\infty(\rho_t),\, \mathbb{1}^{\otimes(r-1)} \otimes \mathrm{d}f(\rho_t)]\Big) \\ &+ \frac{1}{(r-1)! \cdot n^{(r-2)/2}} \cdot \mathrm{Fluct}\Big(i[\mathrm{d}_r H_\infty(\rho_t),\, \mathbb{1}^{\otimes(r-1)} \otimes \mathrm{d}f(\rho_t)]\Big). \end{aligned} \tag{5.39}$$

In the third line, only the terms $(\mathrm{id} - \mathcal{P})^{\otimes r}$ and $(\mathrm{id} - \mathcal{P})^{\otimes(r-1)} \otimes \mathcal{P}$ of $(\mathrm{id} \pm \mathcal{P})^{\otimes r}$ remain, while all other vanish due to the convention (2.39) for the choice of representatives of derivatives $\mathrm{d}_r g(\rho) \in \mathcal{A}$. Therefore, the remaining terms can be written as tensor fluctuators of degree r, resp. $(r-1)$, which leads to the scaling $n^{-(r-1)/2}$, resp. $n^{-(r-2)/2}$ in the last line. That is, in the fluctuator expectation (5.34), the only non-vanishing term is the fluctuator of degree $(r-1)$ for $r = 2$, i.e.

$$\sqrt{n}\,\mathrm{sym}_n\Big(\mathrm{id} \otimes \rho_t\big(i[\mathrm{d}_2 H_\infty(\rho_t),\, \mathbb{1} \otimes \mathrm{d}f(\rho_t)]\big)\Big). \tag{5.40}$$

Hence we can write (5.38) as

$$i[nH_n,\, \widehat{\mathrm{d}f(\rho_t)}] + \frac{\mathrm{d}}{\mathrm{d}t}\widehat{\mathrm{d}f(\rho_t)} = \mathrm{Fluct}\big(\mathrm{d}\{H_\infty, f\}(\rho_t)\big) + O\left(\frac{1}{\sqrt{n}}\right), \tag{5.41}$$

proving the statement. □

In order to prove conjecture 5.3.2, the $O(1/\sqrt{n})$-terms in (5.35) must be sufficiently bounded, such that the integration of (5.34) to finite time intervals can be performed in the limit $n \to \infty$. Although the $O(1/\sqrt{n})$-terms vanish in (5.34), as n tends to infinity, the number of those terms becomes larger and larger for each iterative step of the time evolution. In this project, we did not find a sufficient bound for those terms allowing for the integration to finite time intervals in the infinite-particle limit.

5.4. Time evolution of fluctuators around a mean-field minimizer

In this section, we make the time evolution of fluctuators precise for the case of the reference state ρ being stationary under the mean-field limiting flow $\mathcal{F}_t$. In this case, the fluctuation algebra does not change in time, such that the time evolution of fluctuators is implemented by a Hamiltonian. In particular, we show that if ρ is a minimizer of H_∞, then this Hamiltonian is exactly the fluctuation Hamiltonian $\widehat{H}$, which we used to estimate the $1/n$-corrections of the ground-state energy, cf. Chapter 4.

We assume that the reference state ρ is stationary under the mean-field time evolution, i.e.

$$\dot{\rho} = -i[\mathrm{d}H_\infty(\rho),\, \rho] = 0. \tag{5.42}$$

In this case, the time-evolution equation in the fluctuation algebra, Eq. 5.33, reduces to

$$\begin{aligned}\Big\langle \Omega_t,\, \widehat{\mathrm{d}f(\rho_t)} \cdot \widehat{\mathrm{d}g(\rho_t)} \cdot \ldots \Omega_t \Big\rangle &= \Big\langle \Omega_t,\, \widehat{\mathrm{d}f(\rho)} \cdot \widehat{\mathrm{d}g(\rho)} \cdot \ldots \Omega_t \Big\rangle \\ &= \Big\langle \Omega,\, \widehat{\mathrm{d}f_t(\rho)} \cdot \widehat{\mathrm{d}g_t(\rho)} \cdot \ldots \Omega \Big\rangle,\end{aligned} \tag{5.43}$$

since $\mathrm{d}f(\rho_t) = \mathrm{d}f(\rho)$ for all t. Hence, $\Omega_t \in \mathcal{H}_\rho$. By employing Eq. (5.42), the time derivative of a limiting fluctuator, given by Eq. (5.25), reduces to

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Fluct}_\infty\big(\mathrm{d}f_t(\rho)\big) =& \mathrm{Fluct}_\infty\left(\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{d}f_t(\rho)\right) \\ =& \mathrm{Fluct}_\infty\Big(\mathrm{id} \otimes \rho\left(i\big[\mathrm{d}_2 H_\infty(\rho),\, \mathbb{1} \otimes \mathrm{d}f_t(\rho)\big]\right)\Big) \\ &+ \mathrm{Fluct}_\infty\Big(i\big[\mathrm{d}H_\infty(\rho),\, \mathrm{d}f_t(\rho)\big]\Big).\end{aligned} \tag{5.44}$$

If ρ is additionally a mean-field minimizer of H_∞, then $\widehat{\mathrm{d}H_\infty}(\rho) = 0$ and $\widehat{\widehat{\mathrm{d}H_\infty}}(\rho)$ exists, and the second term in the last line of (5.44) can be written as

$$\mathrm{Fluct}_\infty\Big(i\big[\mathrm{d}H_\infty(\rho),\, \mathrm{d}f_t(\rho)\big]\Big) = i\big[\widehat{\widehat{\mathrm{d}H_\infty}}(\rho),\, \widehat{\mathrm{d}f_t}(\rho)\big], \tag{5.45}$$

by Prop. 3.5.3. For the first term in the last line of (5.44), consider the decomposition

$$\mathrm{d}_2H_\infty(\rho) = \sum_\alpha c_\alpha \otimes c_\alpha, \tag{5.46}$$

using the polarization identity, cf. Lem. 2.5.1. Then we get

$$\begin{aligned}
\big[\widehat{\mathrm{d}_2H_\infty}(\rho),\, \widehat{\mathrm{d}f_t}(\rho)\big] &= \sum_\alpha \big[\widehat{c_\alpha \otimes c_\alpha},\, \widehat{\mathrm{d}f_t}(\rho)\big] \\
&= \sum_\alpha \big[\widehat{c_\alpha} \cdot \widehat{c_\alpha},\, \widehat{\mathrm{d}f_t}(\rho)\big] \\
&= \sum_\alpha \widehat{c_\alpha} \cdot \big[\widehat{c_\alpha},\, \widehat{\mathrm{d}f_t}(\rho)\big] + \big[\widehat{c_\alpha},\, \widehat{\mathrm{d}f_t}(\rho)\big] \cdot \widehat{c_\alpha} \\
&= 2\sum_\alpha \widehat{c_\alpha} \cdot \rho\big([c_\alpha,\, \mathrm{d}f_t(\rho)]\big) \\
&= 2 \cdot \mathrm{Fluct}_\infty\Big(\mathrm{Tr}_2\big(\mathbb{1} \otimes \rho \cdot \big[\sum_\alpha c_\alpha \otimes c_\alpha,\, \mathbb{1} \otimes \mathrm{d}f_t(\rho)\big]\big)\Big) \\
&= 2 \cdot \mathrm{Fluct}_\infty\Big(\mathrm{id} \otimes \rho\,\big(\big[\mathrm{d}_2H_\infty(\rho),\, \mathbb{1} \otimes \mathrm{d}f_t(\rho)\big]\big)\Big),
\end{aligned} \tag{5.47}$$

where in the second line we used the fluctuator decomposition (3.15) and in the fourth line the commutator rule (3.27). Therefore, we see that (5.44) can be written as

$$\frac{\mathrm{d}}{\mathrm{d}t}\widehat{\mathrm{d}f_t}(\rho) = i\big[\widehat{H},\, \widehat{\mathrm{d}f_t}(\rho)\big], \tag{5.48}$$

with the fluctuation Hamiltonian

$$\widehat{H} = \widehat{\widehat{\mathrm{d}H_\infty}}(\rho) + \frac{1}{2}\widehat{\mathrm{d}_2H_\infty}(\rho). \tag{5.49}$$

That is, the time evolution of fluctuators is implemented by the fluctuation Hamiltonian $\widehat{H}$, if ρ is a mean-field ground state.

6. Summary and Outlook

In Part I of this thesis, we introduced the concept of mean field fluctuations and derived their corresponding algebraic structure. In Chapter 3, we showed that the fluctuation method is a powerful tool for estimating $1/n$-corrections to the mean field limit of mean field models in the sense that it allows for a convenient algebraic description in terms of a CCR algebra. Moreover, in Chapter 4 we showed that the $1/n$-corrections to the ground state energy of such models can be obtained by computing the ground state energy of a quadratic Hamiltonian of this CCR algebra. We refined the method to Bosonic mean field models and derived general bounds for the ground state energy of the corresponding fluctuation Hamiltonian. By applying purification techniques we lifted these bounds to general mean field models and, more importantly, showed that every mean field model can be mapped onto a Bosonic one. We applied the theory to two examples from statistical physics, namely the mean field Ising and the Bose-Hubbard model, and to a problem from quantum information theory, namely the finite de Finetti problem. Furthermore, we showed that the Holstein-Primakoff approximation is a special case of the fluctuation method and proposed an extension of the ground state estimation method to a class of approximately symmetric Hamiltonian densities. Finally, in Chapter 5, we provided a conjecture for the time evolution of mean field fluctuations and showed that, under this conjecture, the dynamics of the fluctuations around a mean field minimizer are generated by the corresponding fluctuation Hamiltonian, complementing existing results for mean field models consisting of infinite-dimensional Bosons.

However, there are various open questions remaining. Most importantly, it is not clear whether the fluctuation method gives the optimal $1/n$-corrections to the mean field ground state energy, that is, whether there exists a sequence of true ground states that has root-n fluctuations around a mean field minimizer, cf. Rem. 4.2.4. It was shown before, that this is true under certain conditions for the case of classical mean field models, i.e. where each particle is described by an abelian operator algebra [111]. In order to prove this for quantum mean field models, it is sufficient to obtain a proof for the Bosonic case, cf. Corr. 4.4.8. Furthermore, the bound we obtained for the finite de Finetti problem, cf. Eq. (4.142), is implicit. It would be interesting to derive an explicit bound, depending only on the one-particle dimension d, the particle number k and the degree of exchangability n. If we knew that the $1/n$-corrections are optimal, then this finite de Finetti bound would be optimal, too[1]. On the other hand, if the obtained de Finetti bound would equal the known bound [23] then this would be an indicator that the fluctuation method yields the optimal $1/n$-corrections.

Finally, the concept of mean field fluctuations is not exploited yet and allows for a

[1] The existing bound [23] was shown to be optimal only in the scaling in d, k, and n, but not in the constants.

variety of further applications. For example, it may be possible to estimate first-order corrections of correlation functions. Indeed, given two one-particle observables A and B, then the related correlation function between the particles (i.e. tensor factors) i and j in a permutation invariant state ρ_n an be written as

$$\begin{aligned}\mathrm{Cor}_{\rho_n}(A,B) &= \rho_n\left(A^{(i)}B^{(j)}\right) - \rho_n\left(A^{(i)}\right)\rho_n\left(B^{(j)}\right)\\ &= \rho_n\left(\mathrm{sym}_n(A\otimes B)\right) - \rho_n\left(\mathrm{sym}_n A\right)\rho_n\left(\mathrm{sym}_n B\right),\end{aligned} \tag{6.1}$$

where we assumed $i \neq j$. Hence, if we consider ρ_n as a sequence with root-n fluctuations around a reference state $\rho \in \mathcal{S}(\mathcal{A})$, then we may expand the above strictly symmetric sequences into fluctuators around ρ and obtain

$$\begin{aligned}\mathrm{Cor}_{\rho_n}(A,B) = \frac{1}{2n}\Bigg(&\rho_n\left(\widetilde{\mathrm{d}A_\infty}(\rho)\cdot\widetilde{\mathrm{d}B_\infty}(\rho) + \widetilde{\mathrm{d}B_\infty}(\rho)\cdot\widetilde{\mathrm{d}A_\infty}(\rho)\right)\\ &- 2\rho_n\left(\widetilde{\mathrm{d}A_\infty}(\rho)\right)\rho_n\left(\widetilde{\mathrm{d}B_\infty}(\rho)\right)\\ &-\big(\rho(AB+BA) - 2\rho(A)\rho(B)\big)\Bigg) + O\left(n^{-\frac{3}{2}}\right),\end{aligned} \tag{6.2}$$

where we defined the functions $A_\infty = \mathrm{sym}_\infty A$ and $B_\infty = \mathrm{sym}_\infty B$. Furthermore, by considering the limiting fluctuation algebra $\mathcal{F}_\rho$ with the limiting vector $\Omega \in \mathcal{H}_\rho$ of the sequence ρ_n, we obtain

$$\begin{aligned}\mathrm{Cor}_{\rho_n}(A,B) = \frac{1}{2n}\Bigg(&\left\langle\Omega,\left(\widehat{\mathrm{d}A_\infty}(\rho)\cdot\widehat{\mathrm{d}B_\infty}(\rho) + \widehat{\mathrm{d}B_\infty}(\rho)\cdot\widehat{\mathrm{d}A_\infty}(\rho)\right)\Omega\right\rangle\\ &- 2\left\langle\Omega,\widehat{\mathrm{d}A_\infty}(\rho)\,\Omega\right\rangle\left\langle\Omega,\widehat{\mathrm{d}B_\infty}(\rho)\,\Omega\right\rangle\\ &-\big(\rho(AB+BA) - 2\rho(A)\rho(B)\big)\Bigg) + O\left(n^{-\frac{3}{2}}\right).\end{aligned} \tag{6.3}$$

Two applications can be considered. On the one hand, it may be possible to estimate correlation functions of the ground state of the related mean field model $H_n \in \mathcal{Y}$. If the reference state ρ is a minimizer of H_∞, then the $1/n$-corrections to the ground state energy are given by the ground state of the related fluctuation Hamiltonian $\widehat{H}$. If it is possible to obtain a convenient expression of $\widehat{H}$, as in Sect. 4.5, then one can obtain an expression for Ω as well and compute the related fluctuation expectation values.

On the other hand, it may be possible to compute the time evolution of correlation functions, for example starting from the uncorrelated initial sequence $\rho^{\otimes n}$. By employing the time-evolution equation (5.33), the first-order corrections of the correlation function for the time-evolved state $\rho_{t,n} = \rho^{\otimes n}\circ T_{t,n}$ can be written as

$$\begin{aligned}\mathrm{Cor}_{\rho_{t,n}}(A,B) = \frac{1}{2n}\Bigg(&\left\langle\Omega,\left(\widehat{\mathrm{d}A_{t,\infty}}(\rho)\cdot\widehat{\mathrm{d}B_{t,\infty}}(\rho) + \widehat{\mathrm{d}B_{t,\infty}}(\rho)\cdot\widehat{\mathrm{d}A_{t,\infty}}(\rho)\right)\Omega\right\rangle\\ &- 2\left\langle\Omega,\widehat{\mathrm{d}A_{t,\infty}}(\rho)\,\Omega\right\rangle\left\langle\Omega,\widehat{\mathrm{d}B_{t,\infty}}(\rho)\,\Omega\right\rangle\\ &-\big(\rho_t(AB+BA) - 2\rho_t(A)\rho_t(B)\big)\Bigg) + O\left(n^{-\frac{3}{2}}\right),\end{aligned} \tag{6.4}$$

where Ω is the limiting vector of the initial state at $t = 0$, $\widehat{\mathrm{d}A_{t,\infty}}(\rho)$ and $\widehat{\mathrm{d}B_{t,\infty}}(\rho)$ are the time-evolved fluctuators, and ρ_t is the mean field time-evolved reference state, cf. Eq. (2.46). This may also provide the basis for a comparison of the time evolution of fluctuators, Eq. (5.33), to other popular time-evolution approaches for Bosonic systems beyond mean field, namely the Hartree-Fock-Bogoliubov, -Popov, Griffin or related methods [111], since these are usually implemented as differential equations for two-point correlations, directly from the original Hamiltonian.

Another promising extension of the mean field and fluctuation theory is to relax the permutation invariance. Clearly, many-particle models in condensed matter physics are rarely fully connected but rather contain interactions over finite distances on a lattice. However, it is reasonable to consider local observables, that are influenced only by a small area of that lattice and depend only on a few particles in that area. Since it is not known, which of these particles affect the related expectation value or measurement outcome, it is reasonable to consider the average over all permutations of the observable within the area of interest, i.e. rendering it locally permutation invariant[2]. It is possible to consider a mean field limit in the sense that the area of interest remains constant, but the lattice is made finer and finer, such that it converges to a continuum in the limit. In this limit, it is expected that the set of local observables is described by a classical field theory, i.e. an observable of the type $\mathcal{C}(X, \mathcal{S}(\mathcal{A}))$, which models a mean field algebra at every point x of the continuum X. The related fluctuation algebra is expected to be a Bosonic quantum field theory[3].

[2] A different interesting local mean field theory was developed in [27, 30], where n-particle operators were considered that are permutation invariant over all particles except for a few.

[3] Currently, a related open-science project of this approach from a quantum field-theoretical perspective can be found in https://github.com/tobiasosborne/Continuous-Limits-of-Quantum-Lattice-Systems.

Part II.

Quantum walks with non-orthogonal position states

Notation

$\|\alpha_x\rangle$	Ideal position state, element of a generally non-orthogonal basis in $\ell_2(\mathbb{Z})$, Sect 8.1.
$\|\alpha'_x\rangle$	Vector of the dual basis of $\{\|\alpha_x\rangle\}$, Sect. 10.2.
$\|c_+\rangle$, $\|c_-\rangle$	Ideal coin states, Sect. 8.1.
$\|e_x\rangle$	Vector of an orthonormal basis in $\ell_2(\mathbb{Z})$, Sect. 8.1.
a, a^*	Ladder operators of the axial motional degree of freedom, Sect. 8.2.3.
$\mathbb{C}^2$	Ideal coin space, Sect. 8.1.
$\widetilde{C}\,(\vartheta, \phi)$	Coin transition in experiment, Eq. (8.6).
$C_{\widetilde{\rho_0}}(\lambda)$	Characteristic function, Eq. (10.7).
$C_E = \exp\left(i\,\pi/4\,\sigma_y\right)$	Experimental coin operator Sect 8.1.
$C_H = \sigma_z \cdot C_E$	Hadamard coin operator, Sect 8.1.
$\delta = \omega_z - \omega_L$	Detuning of the optical dipole force from the harmonic oscillator frequency, Sect. 8.2.3.
$\|\Delta\alpha\|$	Step size, Sect 8.1.
$\Delta\Theta$	Increment for momentum shift, Sect. 10.5.
$D\,(\alpha(\tau))$	Coherent-state displacement operator, Sect. 8.2.3.
F_+, F_-	Optical dipole forces on the related coin states, Sect. 8.2.3.
γ	Damping factor in readout process, Sect. 8.2.4.
$g(x)$	Overlap function, Sect 8.1.
$g(p)$	Fourier transform of overlap function.
$\Gamma = \sum_x \|\alpha_x\rangle\,\langle\alpha_x\|$	Gram matrix, Sect. 8.1.
$\mathcal{H} = \ell_2(\mathbb{Z}) \otimes \mathbb{C}^2$	Ideal Hilbert space, Sect 8.1.
$H(\tau)$	Hamiltonian of the ion with the optical dipole force, Sect. 8.2.3.
$H_I(\tau)$	Hamiltonian in the interaction picture, Sect. 8.2.3.
$H_I^{RWA}(\tau)$	Hamiltonian in the interaction picture with the rotating wave approximation, Sect. 8.2.3.

$H_I^{LDA}(\tau)$	Hamiltonian in the interaction picture with the Lamb-Dicke approximation, Sect. 8.2.3.
κ	Component of the wave vector of the optical dipole force in the axial direction z, Sect. 8.2.3.
λ	Wave length of optical dipole force, Sect. 8.2.3.
$\ell_2(\mathbb{Z})$	Ideal position space, Sect 8.1.
$\overline{n} = \mathrm{Tr}(\rho a^* a)$	Mean occupation number of a state ρ in Fock basis, where a^* and a are the ladder operators.
η	Lamb-Dicke parameter, Sect. 8.2.3.
Ω_D	Coupling of the optical dipole force to the ion, Sect. 8.2.3.
$\Omega_{n+1,n} \approx \Omega_{1,0} \cdot \eta\sqrt{n}$	Rabi frequency of the two-photon stimulated Raman transition on the blue sideband, Sect. 8.2.3.
$p_{n,+}$	Probability for the basis state $\|n\rangle \|c_+\rangle$, Sect. 8.2.4.
$P_t(x)$	Probability to find walker at position x after t steps, Sect. 8.1.
$P_\infty(q)$	Asymptotic probability distribution, Sect. 10.3.
$P_+(\tau_B)$	Relative photon-scattering rate in the readout process, Sect. 8.2.4.
$q \in [-1, 1]$	Asymptotic scaled position variable w.r.t. x/t for $t \to \infty$, Sect. 10.3.
$\rho_0 = \|\alpha_0\rangle \langle\alpha_0\| \otimes \rho_{00}$	Ideal initial state, Sect 8.1.
$\rho_{00} = \|c_+\rangle \langle c_+\|$	Coin part of the ideal initial state, Sect 8.1.
$\widetilde{\rho_0}(p)$	Fourier transform of inital state, Sect. 10.3.
$R(\Theta) = \exp(i\,\Theta\,\sigma_z)$	Momentum shift operator, Sect. 10.4.
$\sigma = \sqrt{2}/\|\Delta\alpha\|$	Parameter of overlap function, Sect 8.1.
S	Shift operator, Sect 8.1.
τ_c	Duration of coin pulse, Sect. 8.2.2 .
t	Step number of the nQW, Sect 8.1.
T_p	Pulse duration for photon kick, Sect 9.
$U(\tau)$	Time-evolution operator in the Lamb-Dicke approximation, Sect. 8.2.3.
$v_k(p) = \mathrm{d}\omega_k(p)/\mathrm{d}p$	The kth group velocity, Sect. 10.3.
$V(p) = \sum_k v_k(p) P_k$	Group-velocity operator, Sect. 10.3.
$\omega_k(p)$	The kth eigenstate of $W(p)$, i.e. dispersion relation in p, Sect. 10.3.

ω_{coin}	Rabi frequency of RF driving coin operation.
ω_L	Frequency of optical dipole force, Sect. 8.2.3.
ω_z	Frequency of the axial harmonic oscillator, Sect. 8.2.3.
$W = S \cdot (\mathbb{1} \otimes C)$	Ideal walk operator, Sect 8.1.
$W(p)$	Walk operator in momentum-space, i.e. Fourier transform of W, Sect. 10.3.
z_0	Width of axial ground-state wave function, Sect. 8.2.3.

7. Introduction

Quantum walks (QWs) are a widely used model system for transport processes on lattices. Initially introduced from a computer science perspective [1, 61, 48, 7, 105, 106], the field has significantly expanded and is now largely treated from a physics perspective [34, 74, 87, 79, 2]. In fact, "quantum walk" is now widely taken to be synonymous with "discrete-time or discrete-space quantum dynamics" of a particle with internal degrees of freedom. On a one-dimensional lattice, a QW can always be implemented by a concatenation of coin operations and successive state-dependent shifts [77]. Already these (single-particle) systems are capable of simulating various physical effects such as Anderson localization [4] or the formation of molecules [2]. In particular, single-particle QWs are a basic building block in a bottom-up approach towards general-purpose multi-particle simulation environments [46]. Therefore, one of the main interests in QWs is the possibility to study features of quantum dynamics in a setting which can be controlled experimentally with high precision.

QWs have been experimentally implemented in several different ways, for example using nuclear magnetic resonance [93], atoms in optical lattices [58], trapped ions [101, 72, 125], or photonic systems[1] [16, 103, 20, 83, 84, 99, 81, 96].

In particular, the implementations with trapped ions showed their strengths in the high fidelity of the results. However, these implementations had two major drawbacks. On the one hand, the protocol for the shift operator allowed for a relatively small number of steps, since it worked well only within the so-called *Lamb-Dicke regime* (LDR). On the other hand, the position states, being implemented by coherent states of a harmonic oscillator, were not mutually orthogonal. At the time of the experiments, this was considered as a disadvantage[2] and, in fact, in the theoretical description it was almost universal practice to model the different "positions" by mutually orthogonal subspaces in Hilbert space.

In this part of the thesis, we provide solutions for these drawbacks. On the one hand, we propose a protocol for the shift operator, which is not limited to the LDR and thus allows for a significantly larger number of steps. On the other hand, we present a theoretical model for quantum walks with non-orthogonal position states (nQW) and show that these allow for a variety of interesting experiments. This chapter is organized as follows: In Section 8 we first set up the theoretical framework for an ideal nQW and then describe the experimental details of the implementation with a trapped ion

[1] In the experiments with photonic systems continuous QWs were implemented. In this thesis we do not consider such QWs.

[2] In order to approximate orthogonality in the experiments, the step size was chosen sufficiently large to make these states approximately orthogonal. This in turn further reduced the number of implementable steps.

[101, 72]. In particular, we describe the limitations of the protocol, which allowed for only a few steps of an (orthogonal) QW. Based on this, we propose in Section 9 a new protocol for the implementation of the shift operator of the QW, which is based on photon kicks [39, 40] and not restricted to the LDR. We argue that the photon kicks allow for an implementation of up to 100 steps of a QW with state-of-the-art trapped-ion technology. In Section 10, we present a thorough theoretical treatment of nQWs. By using asymptotic methods [8, 45, 5, 3], we show that the non-orthogonality, which was avoided in the original experiments [101, 72, 125], can be exploited. In particular, we show that the nQW simulates an (orthogonal) QW with an extended initial state. Moreover, we show that state-of-the-art technology allows for manipulating the spreading rate of the QW, probing the dispersion relation of the walk operator, and implementing effects from solid-state physics, such as Bloch oscillations. The results presented in this chapter were published in [72] and [71]. Here, the text closely follows these publications.

8. Preliminaries

8.1. Definitions and theoretical model

In this section, we introduce the ideal model for the non-orthogonal quantum walk (nQW). The notation will be used throughout the chapter. In Section 8.2, we will describe the experimental details of the implementation [101, 72]. There, it is understood that the ideal model is only approximated, although we will use the same notation.

We consider the Hilbert space $\mathcal{H} = \ell_2(\mathbb{Z}) \otimes \mathbb{C}^2$, with $\ell_2(\mathbb{Z})$ being the position space and $\mathbb{C}^2$ the coin space. The (normalized but not mutually orthogonal) position states $|\alpha_x\rangle$, with $x \in \mathbb{Z}$, form a basis of $\ell_2(\mathbb{Z})$. The coin states $|c_+\rangle$ and $|c_-\rangle$ are the eigenstates of the Pauli matrix σ_z. We assume the initial state of the nQW to be localized at the origin, i.e., $\rho_0 = |\alpha_0\rangle\langle\alpha_0| \otimes \rho_{00}$ with $\rho_{00} = |c_+\rangle\langle c_+|$.

One step of the nQW is given by the application of the walk operator $W = S \cdot (\mathbb{1} \otimes C)$, which is composed of a unitary coin operator C and a unitary shift operator S. The latter acts as

$$S\,|\alpha_x\rangle \otimes |c_\pm\rangle = |\alpha_{x\pm1}\rangle \otimes |c_\pm\rangle\,. \tag{8.1}$$

In fact, the position states $|\alpha_x\rangle$ are defined by the subsequent application of S on $|\alpha_0\rangle$. It follows that their overlap $\langle\alpha_x|\alpha_y\rangle$ is translation invariant. In the spirit of the trapped-ion system, the position states model coherent states of a continuous-variable system, namely a motional degree of freedom of the ion. Hence, we define the overlap function

$$g(x) = \langle\alpha_0|\alpha_x\rangle = \exp(-x^2/\sigma^2), \tag{8.2}$$

where $\sigma = \sqrt{2}/|\Delta\alpha|$ determines the overlap between different position states and the step-size $|\Delta\alpha|$ is the distance of the related neighbouring coherent states in the phase space of the continuous variable system, cf. Fig. 8.1.

The projector $F_x = |\alpha_x\rangle\langle\alpha_x|$ is used to model the probability to find the walker at position $|\alpha_x\rangle$ after t steps [101, 72]. That is,

$$P_t(x) = \frac{\mathrm{Tr}\Big(\big(F_x \otimes \mathbb{1}\big) \cdot W^t \rho_0 W^{-t}\Big)}{\mathrm{Tr}\big(G \cdot \rho_0\big)}, \tag{8.3}$$

where $G = \Gamma \otimes \mathbb{1}$ with $\Gamma = \sum_x F_x$ being the Gram matrix, yielding a normalized probability distribution. Note that $[S, G] = 0$, due to the unitarity of S, such that the normalization is independent of the step number t.

For the coin operator, we consider two cases. On the one hand, we define the coin operator $C_E = \exp(i\,\pi/4\,\sigma_y)$. This one has been implemented experimentally with the

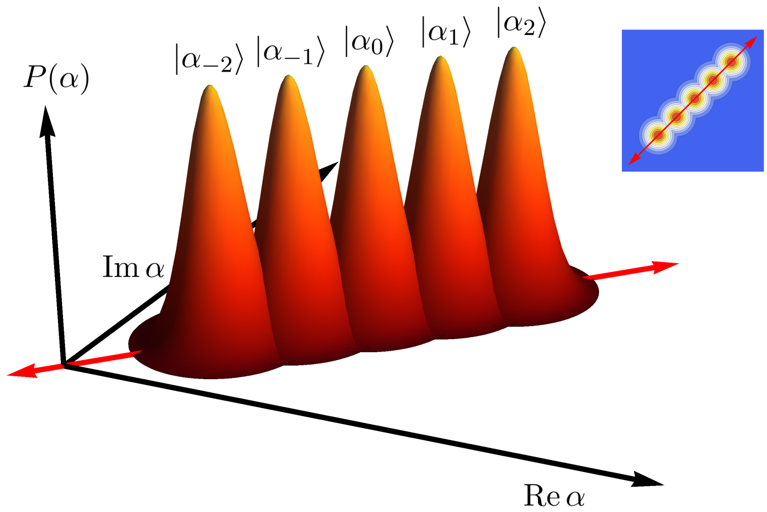

Figure 8.1.: nQW implemented in the phase space of a harmonic oscillator. The position states $|\alpha_x\rangle$ are coherent motional states, illustrated in the figure by their Husimi functions, $P_x(\alpha) = |\langle\alpha|\alpha_x\rangle|^2$, for $x = -2, -1, \dots, 2$. The inlay illustrates their orientation in phase space, implementing a nQW along a line. Since the position states $|\alpha_x\rangle$ are coherent states, they are not mutually orthogonal. The step size $|\Delta\alpha|$ (cf. Eq. (8.2)) of the nQW determines the overlap between different position states. QWs of this type have been implemented with trapped ions [101, 72, 125]. Figure and caption from [71].

initial state ρ_0 [101, 72, 125]. We will refer to it as the experimental walk[1]. The other coin operator is the Hadamard matrix $C_H = \sigma_z \cdot C_E$. The position-probability distributions of nQWs with the coin operators C_E and C_H are illustrated in Fig. 8.2. The coin operators C_E and C_H are similar, in the sense that the probability distributions are equal in the orthogonal case ($\sigma = 0$). In contrast, they show significantly different behaviour in the case of large overlaps ($\sigma \gtrsim 1$).

8.2. Experimental implementation

In this section, we outline the experimental implementation of the quantum walk (QW) [101, 72]. Although the position states were implemented in the form of coherent states of a harmonic oscillator, which are mutually non-orthogonal, the step size $|\Delta\alpha|$ was set large enough to restore approximate orthogonality, which in turn severly reduced the number of steps. In the following, we review the experimental details, closely following the description in [72]. We focus on the limitations of the optical dipole force implementing of the shift operator. In Section 9, we will propose a protocol for the shift-operator implementation via photon kicks, which is not bound by these limitations and therefore allows for a significantly higher number of steps.

8.2.1. The ion

The QW was implemented with a $^{25}\mathrm{Mg}^{+}$ ion, confined in a linear Paul trap [98]. Two hyperfine states were defined to be the coin states, namely

$$|c_-\rangle \equiv \left|{}^2S_{1/2}, F = 2, m_F = 2\right\rangle \text{ and} \tag{8.4}$$

$$|c_+\rangle \equiv \left|{}^2S_{1/2}, F = 3, m_F = 3\right\rangle. \tag{8.5}$$

The hyperfine states were separated in energy by a Zeeman shift induced from a static magnetic field. This allowed for selectively adressing each hyperfine state via a microwave field, as will be described in the next subsection. The motional degree of freedom in the axial direction, which admits a harmonic motion for low amplitudes, served as the space in which the position states were implemented in the form of coherent motional states.

The experimental protocol for the QW, i.e. one experimental cycle, consists of several steps: (1) initialization, (2) implementation of the QW and (3) state readout. The whole experiment consisted of a few 1000 such cycles for each set of parameter values in order to obtain the required statistical relevance. In the following, we describe the building blocks for one cycle. A concise discussion of these tools in a generic context can be found in [122] and [65].

At the beginning of each experimental cycle, the ion was initialized in the coin state $|c_+\rangle$ with a fidelity ≥ 0.99 by optical pumping [75], while the motion of the ion was cooled close to the ground state by Doppler cooling (with a mean occupation $\overline{n} \approx 10$) [121] in the eigenbasis of the harmonic oscillator in each direction. The axial motion was further cooled by sideband cooling to $\overline{n} < 0.03$ [75], i.e. effectively to the ground state.

[1]Not implying that C_H, the other coin operator, cannot be implemented experimentally

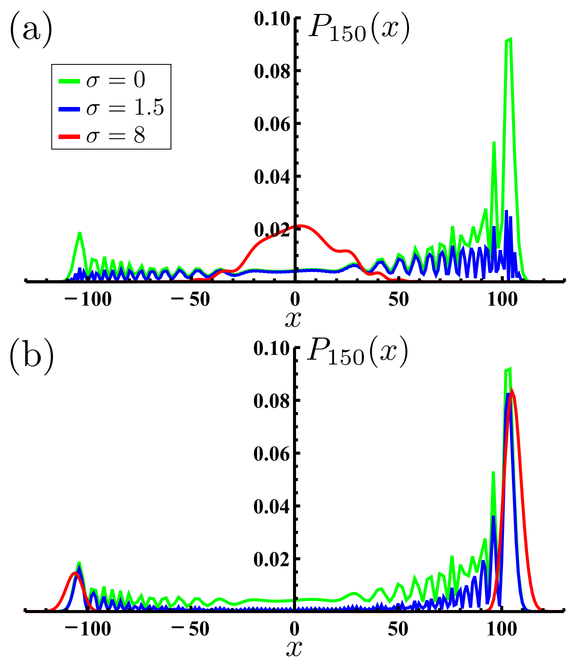

Figure 8.2.: Position-probability distribution $P_t(x)$ (8.3) after $t = 150$ steps of a nQW with overlap function $g(x)$ (8.2) and (a) the experimental coin C_E and (b) the Hadamard coin C_H for $\sigma = \{0, 1.5, 8\}$ (green, blue, red). (For the green curve, only points x with $P(x) \neq 0$ are connected.) In the orthogonal case (green) the probability distributions of both types of walks are equal, however for large overlaps they differ significantly (blue, red). In case (a), the probability distribution approaches a Gaussian shape centered at the origin of the walk, as σ is increased. The spreading, which is still linear in the step number t, is vastly reduced [72]. In the Hadamard case (b), the probability distribution approaches a shape consisting of two Gaussian peaks centered around $\pm t/\sqrt{2}$. Thus, the (linear) spreading is increased, as the probabilities between the peaks vanish. The initial state is $\rho_0 = |\alpha_0\rangle\langle\alpha_0| \otimes |c_+\rangle\langle c_+|$. Figure and caption from [71].

8.2.2. The coin operator

Transitions between the coin states were achieved by applying a radio-frequency field (RF) on resonance with the energy separation between $|c_+\rangle$ and $|c_-\rangle$, given by the frequency ω_{coin}, for a duration τ_c [122]. This implements the operator

$$\widetilde{C}\,(\vartheta,\phi) = \begin{pmatrix} \cos(\vartheta/2) & e^{i\phi}\sin(\vartheta/2) \\ -e^{-i\phi}\sin(\vartheta/2) & \cos(\vartheta/2) \end{pmatrix} \tag{8.6}$$

on the coin space with $\vartheta = \Omega\cdot\tau_c$ and Ω being the Rabi frequency of the transition. The coin operator C_E was implemented by setting $\vartheta = \pi/2$, since $C_E = \widetilde{C}(\pi/2, 0)$. The phase ϕ, which is uncontrolled for the first pulse, was set constant for all coin operations within one experimental cycle, such that it does not influence the probability distribution. The duration of a coin operation, or more generally the duration of one experimental cycle was well within the coherence time of the RF field, such that dephasing of the coin operation (w.r.t. ϕ) was negligible. Spin-echo sequences [122], which were included in the QW pulse sequence, further reduced this issue.

8.2.3. The shift operator

The shift operator S was implemented by a coin-state dependent optical dipole force. It was the limiting factor for the number of steps of the QW, because at large amplitudes a severe deviation from the ideal model occurred. In the following, we will describe this issue more precisely.

The initial motional state after sideband cooling was close to the ground state $|n = 0\rangle$, with a mean occupation $\overline{n} < 0.03$. A coin-state dependent optical dipole force, acting into the axial direction of the trap and oscillating with frequency ω_L with a phase separation of π between the coin states, was implemented by applying a two-photon stimulated Raman transition between the coin states via the $P_{3/2}$ orbital state manifold, using two laser beams [122]. The frequency difference between the lasers was ω_L and the wave vectors were such that the effective wave vector of the Raman transition was directed into the axial direction of the Paul trap.

In a simplified picture, the two laser beams provide a walking standing wave of a coin-state dependent AC-Stark shift. This creates the forces F_+ and F_- on the coin states $|c_+\rangle$ and $|c_-\rangle$, proportional to the spatial gradient of the walking wave and oscillating with frequency ω_L. The ratio of the forces acting on the coin states amounts to $F_-/F_+ \approx -2/3$. The polarizations and intensities of the laser beams are adjusted such that the time-averaged AC-Stark shift, which would cause a dephasing of the coin operations, is negligible for the relevant pulse durations [120]. The effective wavelength of the walking wave amounts to $\lambda \approx 200$ nm. With the width of the axial ground-state wave function of $z_0 \approx 10$ nm, this results in a Lamb-Dicke parameter of $\eta = z_0\cdot 2\pi/\lambda = 0.31$ [122].

The Lamb-Dicke parameter determines, up to which motional amplitude the dynamics resulting from the optical dipole force can be described by a displacement operator. To obtain the latter, two approximations must hold for the dynamics: The rotating wave approximation (RWA) and the Lamb-Dicke approximation (LDA). The area in the motional phase space, in which the LDA holds, is called the Lamb-Dicke regime (LDR). With the optical dipole force, it is only possible within the LDR to implement the step operator S. In the following, we outline the application of these approximations to the Hamiltonian and the related dynamics.

We consider the following time-dependent Hamiltonian describing the effective two-level system (coin) coupled to the harmonic oscillator (axial motion) and interacting with the optical dipole force, modeled by a classical light field with frequency ω_L, wave-vector component κ in the axial direction z and coupling factor Ω_D [122],

$$\begin{aligned} H(\tau) =& H_{coin} + H_{motion} + H_{interaction}(\tau) \\ =& \frac{1}{2}\hbar\omega_{coin}\sigma_z + \hbar\omega_z\left(a^*a + \frac{1}{2}\right) + \frac{\hbar}{2}\left(e^{i(\eta(a+a^*)-\omega_L\tau+\phi_0)} + h.c.\right) \otimes \underline{\Omega}_D, \end{aligned} \tag{8.7}$$

where ω_{coin} is the frequency of the energy separation between $|c_+\rangle$ and $|c_-\rangle$, ω_z is the frequency of the axial harmonic oscillator and $\underline{\Omega}_D = \Omega_D\left(|c_+\rangle\langle c_+| - \frac{2}{3}|c_-\rangle\langle c_-|\right)$. σ_z denotes the Pauli z-matrix and a, a^* are the ladder operators of the harmonic oscillator in the axial direction. In the interaction picture, with the free Hamiltonian being $H_{coin} + H_{motion}$, the interaction Hamiltonian can be written as

$$\begin{aligned} H_I(\tau) =& \frac{\hbar}{2}\sum_{m=0}^{\infty}\sum_{n=0}^{\infty} |m\rangle\langle m| e^{i\eta(a+a^*)}|n\rangle\langle n| \\ &\times\left(e^{i((m-n)\omega_z-\omega_L)\tau+i\phi_0} + (-1)^{|m-n|}e^{i((m-n)\omega_z+\omega_L)\tau-i\phi_0}\right)\otimes\underline{\Omega}_D. \end{aligned} \tag{8.8}$$

If the dipole force is applied with a small detuning of $\delta = \omega_z - \omega_L$, such that the terms corresponding to first-sideband transitions, $|n\rangle \leftrightarrow |n+1\rangle$, rotate slowest and thus dominate, then it is sufficient to consider only those, i.e. to apply the RWA. The interaction Hamiltonian is then reduced to:

$$\begin{aligned} H_I^{RWA}(\tau) =& \frac{\hbar}{2}\sum_{n=0}^{\infty}\Big(\langle n+1| e^{i\eta(a+a^*)}|n\rangle e^{i(\delta\tau+\phi_0)}\cdot|n+1\rangle\langle n| \\ &- \langle n| e^{i\eta(a+a^*)}|n+1\rangle e^{-i(\delta\tau+\phi_0)}\cdot|n\rangle\langle n+1|\Big)\otimes\underline{\Omega}_D. \end{aligned} \tag{8.9}$$

For states with $\eta\sqrt{\langle(a+a^*)^2\rangle} \ll 1$, we can perform the Lamb-Dicke approximation (LDA) [122], i.e.

$$\langle n+1| e^{i\eta(a+a^*)}|n\rangle \approx i\eta\sqrt{n+1}. \tag{8.10}$$

That is, the potential providing the dipole force changes linearly over the extension of the wave function. We can then simplify the interaction Hamiltonian to

$$H_I^{LDA}(\tau) = \frac{i\eta\hbar}{2}(a^*e^{i(\delta\tau+\phi_0)} - ae^{-i(\delta\tau+\phi_0)})\otimes\underline{\Omega}_D. \tag{8.11}$$

In the following, we set $\hbar = 1$ and $\phi_0 = 0$, as ϕ_0 represents the initial phase relation between ion motion and dipole force, which does not influence the results of the QW.

The time-evolution operator resulting from $H_I^{LDA}(\tau)$ has been solved analytically [22] and can be written as

$$U(\tau) = |c_+\rangle\langle c_+| \otimes D\left(\alpha(\tau)\right) \cdot e^{i\Phi(\alpha(\tau),\tau)} + |c_-\rangle\langle c_-| \otimes D\left(-\frac{2}{3}\alpha(\tau)\right) \cdot e^{i\Phi\left(-\frac{2}{3}\alpha(\tau),\tau\right)}, \quad (8.12)$$

where $D\left(\alpha(\tau)\right)$ is the coherent-state displacement operator and

$$\Phi\left(\alpha(\tau),\tau\right) = \mathrm{Im}\left(\int_0^\tau \mathrm{d}s\, \alpha^*(s) \frac{\mathrm{d}\alpha(s)}{\mathrm{d}s}\right). \quad (8.13)$$

The factor 2/3 in (8.12) results from the difference of the state-dependent dipole force, $F_-/F_+ = -2/3$, which is just a property of the experimental setup used in [72]. The complex parameter $\alpha(\tau)$ amounts to

$$\alpha(\tau) = \frac{\eta\Omega_D}{2} \cdot \int_0^\tau e^{i\delta\tau} \mathrm{d}\tau = -i\frac{\eta\Omega_D}{2\delta} \cdot \left(e^{i\delta\tau} - 1\right) \quad (8.14)$$

and corresponds to a circular trajectory in a co-rotating phase space. In Fig. 8.3, the time evolution under the optical dipole force is illustrated. Clearly, at a certain motional amplitude the LDA breaks down in the sense that it does not describe the correct trajectory, which severely deviates from a circular one and causes *motional squeezing* [73, 72].

The shift operator S was implemented by the application of the dipole force for a duration that corresponds roughly to a semi-circular trajectory of the state within the LDA, while the force ratio F_+/F_- was compensated by a type of spin-echo sequence, as illustrated in Fig. 8.4. The precise duration for the dipole-force pulses was optimized experimentally to maximize the asymmetry of the position probabilities at $x = 1$ and $x = -1$ after three steps.

Clearly, the optical dipole force was the limiting factor for both, the quality of the implementation of the QW and the number of implementable steps. A similar implementation of a QW was reported in [125]. There, the number of steps was 23 instead of three, which was partly possible due to a much lower Lamb-Dicke parameter in their experimental setup.

8.2.4. State readout

The state readout was performed by driving the cycling transition

$$|n\rangle|c_+\rangle \rightarrow |n\rangle\left|2P_{3/2}, F = 4, m_F = 4\right\rangle \quad (8.15)$$

for all n and detecting the scattered photons with a photomultiplier, yielding the probability of the coin state $|c_+\rangle$. To readout the motional state, the following scheme was implemented: First, the population on the state $|n\rangle|c_-\rangle$ was transfered to an isolated state $|n\rangle|A\rangle$ (for all n) by appropriate RF pulses. Then a two-photon stimulated Raman transition $|n\rangle|c_+\rangle \leftrightarrow |n+1\rangle|c_-\rangle$ (i.e. on the *blue sideband*), for all n, was performed for a variable pulse-duration τ_B. The Rabi frequencies for these transitions amount to

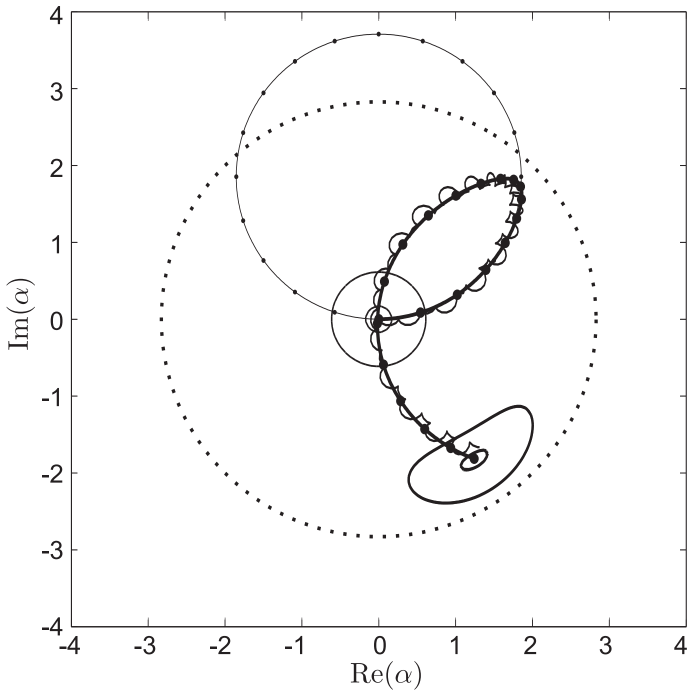

Figure 8.3.: Numerical simulation of the ion trajectory in co-rotating phase space (where the free evolution is eliminated), driven by the dipole force in the full model (with up to 3 sidebands) (8.8), RWA (8.9) and LDA (8.11). The initial state is at the origin ($|\alpha_0 = 0\rangle$). The thin concentric lines represent contours of its Wigner function W (at $W_> = 0.6$ and $W_< = 0.3$). The bold dotted line represents the limit of the LDR, which lies approximately at the Fock state $g_1 = 8$. The thin circular trajectory with dots represents the result of the simulation within the LDA. The dots on the trajectory depict the positions after $\tau = 0, 0.5, ...10$ µs. The final state, reached after $T_{2\pi} = 2\pi/\delta = 10$ µs, equals the initial one, up to a phase factor. The bold trajectory represents the result within the RWA, taking nonlinearities of the dipole force into account. The dots on the trajectory again depict the position at the times $\tau = 0, 0.5, ...10$ µs. Starting from the origin, the trajectory is identical to the one within the LDA. Close to the boundary of the LDR, the trajectories start to deviate. The acceleration of the ion ceases at a certain amplitude, the state gets squeezed and then returns to the origin after a duration shorter than $T_{2\pi}$. The spiraling trajectory, which follows the one within the RWA, represents the results of the full model (with up to 3 sidebands). Here, terms of higher frequencies in the Hamiltonian cause the spiralling. The final Wigner function is almost identical to the one in the RWA and therefore not shown. Parameters: $\Omega_D = 2\pi \cdot 1.2$ MHz, $\omega_L = 2\pi \cdot 2.03$ MHz, $\omega_z = 2\pi \cdot 2.13$ MHz, $\eta = 0.31$, $t \in [0, 10]$ µs. Figure and caption from [72].

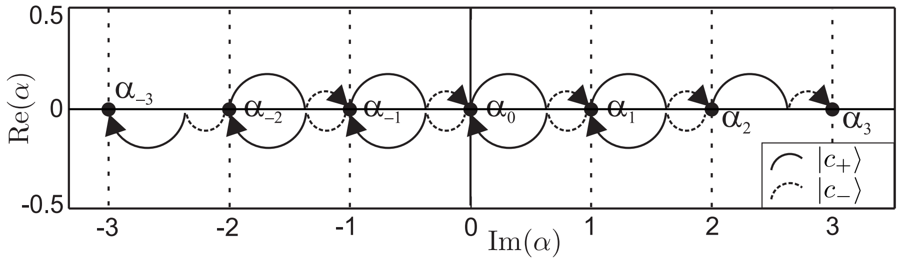

Figure 8.4.: Ideal implementation of the QW in the co-rotating phase space (where the free evolution is eliminated). Starting from position $|\alpha_0\rangle$ and a superposition of the coin states (from the first coin operation), the optical dipole force transfers the motional state for each coin state to the left or right, clock-wise along a semi-circular trajectory (dotted and solid line). Since the values of the forces F_+ and F_- are different, the coin states are swapped after a semi-circular evolution by an RF pulse, and the dipole force is applied a second time for a semi-circular evolution to complete the shift to $|\alpha_{-1}\rangle$, resp. $|\alpha_1\rangle$. The subsequent application of these pulses implements the QW within the LDR. Figure from [72].

$\Omega_{n+1,n} \approx \Omega_{1,0} \cdot \eta\sqrt{n}$ within the LDR and therefore depend on the eigenstates $|n\rangle$ of the harmonic oscillator. The measured probability therefore amounts to [122]

$$P_+(\tau_B) = \frac{1}{2}\left(1 + \sum_{n=0}^{\infty} p_{n,+} \cdot \cos(\Omega_{n+1,n} \cdot \tau_B) e^{-\gamma \cdot \tau_B}\right), \tag{8.16}$$

where $p_{n,+}$ is the probability for the basis state $|n\rangle|c_+\rangle$ after the QW. The damping factor γ accounts for decoherence effects [122]. A discrete Fourier transformation of (8.16) allows to access the probabilities $p_{n,+}$. By exchanging the populations on $|c_+\rangle$ and $|c_-\rangle$ via an appropriate RF pulse before the readout process, the probabilities $p_{n,-}$ were obtained.

Via a comparison with a numerical simulation and some further readout operations (i.e. performing another shift operation on the final state), the idealized probabilities $P_t(x)$, after t steps of the QW, (8.3) were obtained [72].

8.2.5. Limits of the implementation

In [101, 72] the feasibility of implementing a QW with a trapped ion was demonstrated. In particular, the strength of the ion-system was revealed to be the high fidelity of the results. While the quality of the coin operation allows for a significantly higher number of steps, the limiting factor of the step number was the Lamb-Dicke parameter $\eta = 0.31$ of the optical dipole force. In a similar experiment [125], the step number was much higher (23 instead of three), which was partly possible due to a much lower Lamb-Dicke parameter. Reducing the Lamb-Dicke parameter further was argued not to be promising [72].

Conclusively, the main limitations of the experiments [72, 125] are, on the one hand, the implementation of the shift operator, being limited by the Lamb-Dicke regime, and on the other hand, the desire of making the position states approximately orthogonal.

In the next sections, we propose two extensions of the experiments. On the one hand, we propose a method for the implementation of the shift operator, that is not limited to the Lamb-Dicke regime and therefore in principle allows for a vastly higher number of steps. On the other hand, we investigate the influence of non-orthogonality of the position states on the QW, which was partially observed in [72], but avoided in the experiment. We show that the non-orthogonality can be exploited and allows for a variety of interesting experiments, namely the simulation of QWs with extended initial states, controlling the spreading rate of the QW, probing the walk operator experimentally and simulating Bloch oscillations. These experiments can be readily implemented using state-of-the-art technology and even allow for a much higher step number, since the step size $|\Delta\alpha|$ is much lower.

9. Implementing the shift operator with photon kicks

In this section, we describe the implementation of the shift operator with photon kicks [39, 40], which we proposed in [72] and which is substantially less dependent on the motional state and allows for the implementation of QWs with many steps. This section closely follows the corresponding chapter in [72]. The principle of a photon kick is to apply a π-pulse on the coin states with a sufficiently short duration, such that the free harmonic motion of the ion during the pulse is negligible. It was shown that the change of the momentum of the ion during such a pulse can be described by a displacement operator, allowing us to propose its application as a building block for the shift operator of a QW. In the original protocol [39], implemented in [21], however, the influence of the motional state on the performance of the photon kicks has not been considered, since the amplitudes of the motional states were assumed to remain small. For the implementation of a QW with many steps, we have to consider (coherent) motional states with very large amplitude and thus have to re-assess the validity of the above-mentioned approximation. We find that, for a given fidelity, the upper bound for the pulse duration scales inversely with the motional amplitude, and additionally, for coherent motional states, depends on the phase of their harmonic oscillation at the moment when the pulse is applied. In the following we derive an analytic bound for general states and present the results of a numerical study for coherent motional states. With the latter, we show that QWs with up to 100 steps for a step size of $|\Delta\alpha| = 2$ should be possible with state-of-the-art technology.

As above, we consider for our system a harmonic oscillator coupled to a 2-level system and being under the influence of a classical light field. Referring to [39], we start our analysis with the Hamiltonian

$$\begin{aligned} H &= H_0 + H_1 \\ &= \frac{\Omega}{2}\left(e^{i\eta(a^\dagger + a)} \otimes \sigma_+ + e^{-i\eta(a^\dagger + a)} \otimes \sigma_-\right) + \omega_z a^\dagger a \otimes \mathbb{1}, \end{aligned} \tag{9.1}$$

where Ω is the coupling parameter for the light field and $\sigma_\pm = (\sigma_x \pm i\sigma_y)/2$.

This Hamiltonian can be implemented in various ways, e.g. via direct dipole coupling, two-photon stimulated Raman transitions or stimulated Raman adiabatic passage [39]. Each implementation imposes different constraints on pulse duration, laser intensities, etc. In the following, we will focus on the implementation with a two-photon stimulated Raman transition and consider the energy levels of $^{25}Mg^+$.

In this configuration, two laser beams (R_a,R_b) resonantly drive two-photon transitions between the coin states via a virtual state detuned from the $P_{3/2}$ state manifold by Δ_R.

Each laser beam drives only one of the two Raman branches, due to their different polarizations. In a RWA, terms varying at optical frequencies are neglected. This is valid in our case for pulse durations well above $1/10^{-15}$ Hz = 1 fs. Finally, an adiabatic elimination of the $P_{3/2}$ states requires $|\Omega/\Delta_R| \ll 1$. The pulse duration T_p in our case must therefore be sufficiently longer than 5 ps for $\Delta_R \approx 2\pi \cdot 10^{11}$ Hz and $T_p\Omega = \pi$ (see below). The effective wave vector of the two-photon transition is $\kappa = \kappa_a - \kappa_b$.

Hamiltonian (9.1) implements the desired displacement operator for a pulse duration of $T_p = \pi/\Omega$, if we neglect the perturbation H_1. The related unitary transformation amounts to

$$\begin{aligned} U_0(T_p) =& e^{-iH_0 T_p} \\ =& \cos\left(\frac{\Omega T_p}{2}\right) \cdot \mathbb{1}_{motion} \otimes \mathbb{1}_{coin} \\ &- i \sin\left(\frac{\Omega T_p}{2}\right) \cdot \big(D(i\eta) \otimes \sigma_+ + D(-i\eta) \otimes \sigma_- \big) \\ =& - i \big(D(i\eta) \otimes \sigma_+ + D(-i\eta) \otimes \sigma_- \big), \end{aligned} \tag{9.2}$$

which is obtained by expanding the exponential function, splitting the series into odd and even parts and using the properties of the Pauli matrices and displacement operators.

The shift operator itself, implementing the step size $|\Delta\alpha| = 2$ for an orthogonal QW, can be realized by the subsequent application of $2/\eta$ kicks in such a way that the displacements $D(i\eta)$ of several π-pulses add up to $D(i|\Delta\alpha|)$. This can be achieved by changing the direction of the effective wave vector by 180° for each photon kick. In practice one can either switch between two Raman beam configurations with opposite effective wave vectors, or implement every second π-pulse by a RF transition for which the momentum transfer is negligible. Notably, with this protocol the step sizes for both directions of the QW are equal, in contrast to the method of optical dipole forces used in the trapped-ion experiment described above.

In the following, we derive a conservative estimate for the deviation from a coherent-state displacement induced by H_1. The total time-evolution operator amounts to

$$U(\tau) = e^{-iH\tau} = U_0(\tau) \cdot V(\tau) \tag{9.3}$$

with $V(\tau) = e^{iH_0\tau} e^{-iH\tau}$. $V(\tau)$ can be differentiated

$$\dot{V}(\tau) = -ie^{iH_0\tau} H_1 e^{-iH_0\tau} \cdot V(\tau), \tag{9.4}$$

leading to an equation, which is formally solved by the integral equation

$$V(\tau) = \mathbb{1} - i \int_0^\tau \mathrm{d}s \; e^{iH_0 s} H_1 e^{-iH_0 s} \cdot V(s), \tag{9.5}$$

using $V(0) = \mathbb{1}$. Consider the norm-distance ϵ between the evolved state according to the full Hamiltonian and the desired evolved state according to H_0:

$$\begin{aligned} \epsilon \equiv& \left\| (U(\tau) - U_0(\tau)) |\psi\rangle \right\| \\ =& \left\| (V(\tau) - \mathbb{1}) |\psi\rangle \right\| \\ =& \left\| \int_0^\tau \mathrm{d}s \; e^{iH_0 s} H_1 e^{-iH_0 s} V(s) |\psi\rangle \right\|. \end{aligned} \tag{9.6}$$

Approximating the last expression by the largest term of the first-order Dyson series and considering a motional state $|\psi\rangle = |\alpha\rangle |c_-\rangle$, we find the following error estimate for a pulse with duration T_p [39]

$$\epsilon \approx \left\| \int_0^{T_p} \mathrm{d}s \ \omega_z (\mathbb{1} \otimes a^\dagger a) |\psi\rangle \right\| = T_p \omega_z |\alpha|^2. \tag{9.7}$$

Thus, for an initial state $|\alpha\rangle |c_-\rangle$ (the coin state can be chosen arbitrarily), the pulse duration T_p necessary to implement the displacement operator with an error smaller than ϵ must fulfill

$$T_p \leq \frac{\epsilon}{\omega_z \cdot |\alpha|^2}. \tag{9.8}$$

The scaling with $|\alpha|^{-2}$ is, however, a rather rough estimate. This is shown by a numerical simulation of this process, in particular considering the application of photon kicks to (superpositions of) coherent motional states. We compute the fidelity $f = |\langle\alpha| \langle c_-| U_0^\dagger(T_p) U(T_p) |\alpha\rangle |c_-\rangle|^2$ with the initial state $|\alpha\rangle |c_-\rangle$, a pulse duration T_p, and $\Omega = \pi/T_p$, where the time evolution is implemented using a Runge-Kutta method. The results show that the fidelity strongly depends on the phase of the ion oscillation at the moment of the photon kick.

Demanding a fidelity of $f \geq 0.99$ and for imaginary α, i.e. at the moment of the photon kick the ion is in the center of the harmonic potential and thus fastest, for the experimental parameters from [72], we find[1]

$$T^{\mathrm{Im}}_{f=0.99}(|\alpha|) = \exp\left(-17.55 - 0.63 \ln(|\alpha|) - 0.05 \left(\ln\left(|\alpha|\right)\right)^2\right). \tag{9.9}$$

For $|\alpha| = 200$, the amplitude reached after the 100th step of a QW with $|\Delta\alpha| = 2$, the pulse duration must be shorter than $T^{\mathrm{Im}}_{f=0.99}(200) = 0.21$ ns.

However, applying the photon kick at a time at which the ion is at its turning point, i.e. when the ion is slowest and α is real, the scaling is less demanding. We find

$$T^{\mathrm{Re}}_{f=0.99}(|\alpha|) = \exp\left(-17.03 - 0.02 \ln(|\alpha|) - 0.1 \left(\ln\left(|\alpha|\right)\right)^2\right). \tag{9.10}$$

Most importantly, the prefactor of the term linear in $\ln(|\alpha|)$ is much smaller than for an imaginary α. For the 100th step, the pulse duration therefore only has to be shorter than $T^{\mathrm{Re}}_{f=0.99}(200) = 2.18$ ns, which is within the specifications of a fast-switching electro-optic modulator and the continuous-wave laser system used in [72]. Timing the application of the photon kick to the (spatial) turning points of all the coherent oscillations occuring during the QW is possible, because we start the QW in the motional ground state and the position states are aligned along a line in the co-rotating phase space. Thus, coherent states of different $|\Delta\alpha|$ reach their turning points simultaneously.

If the width of the ground-state wave function amounts to $z_0 = 10$ nm, then the coherent motional state $|\alpha_{max} = 200\rangle$ has a real-space amplitude of 4 µm. At such high motional amplitudes anharmonicities of the trapping potential must be considered. These

[1] Equations (9.9) and (9.10) are the results of quadratic fits to double-logarithmic plots of pairs $(T_p, |\alpha|)$ for a fidelity $f = 0.99$ and $|\alpha| \leq 10$. Higher motional amplitudes were not considered due to sizable additional numerical effort. For the following estimates, the scaling is considered to be preserved.

depend on the design of the electrodes and could be eliminated, e.g. by designing the Paul trap electrodes in a hyperbolic shape [82]. Additionally, micromotion [122] might increase the deviation from the ideal walk, for example by reducing the overlap of the additionally oscillating motional wave functions. However, it will remain negligible when the QW is implemented in the axial degree of freedom of an ion in a linear Paul trap.

A major challenge, but also an interesting research topic on its own, is the consideration of decoherence processes, in particular heating and dephasing of the motional state, especially at the large motional amplitude occuring during the QW. Several studies, theoretical [116] and experimental [26, 76], have been performed in the past. To estimate the amount of decoherence, one can consider a Ramsey-interferometry experiment incorporating a Schrödinger-cat state consisting of the two outermost states $|\alpha_{100}\rangle$ and $|\alpha_{-100}\rangle$, and estimate the expected decay of the Ramsey fringes. This has experimentally been found to scale as $\exp(-d^2\lambda\tau)$ [76], where $d = |\alpha_{100} - \alpha_{-100}|$ is the distance between the coherent states in phase space, τ the time needed to create both states and λ representing the scaling parameter incorporating heating and dephasing. Using a Paul trap with hyperbolically shaped electrodes to ensure a harmonic confinement, implies a large electrode-ion distance on the order of millimeters. This reduces heating by several orders of magnitude compared e.g. to the setup used in reference [26], where the dependence of heating to the electrode-ion distance has been investigated. Additionally, cooling the electrodes to cryogenic temperatures, which further reduces the heating rate [26], is currently becoming state-of-the-art technology in trapped-ion experiments. Dephasing, on the other hand, depends mainly on the stability of the trap frequency ω_z against fluctuations. We believe that a lot of improvement is possible by extensive use of stabilization electronics, which has not been brought to the edge of the technically possible, yet, since large motional amplitudes have not been a major issue in most experiments. In fact, our experiment of the three-step QW required an improved frequency stabilization which was achieved to a sufficient amount by a simple electronic circuit. It remains to consider the duration τ, which, using the photon-kick protocol, is about one order of magnitude longer compared to [76]. However, the duration of the coin toss, being the constituent of longest duration in the protocol, can be reduced to a pulse duration of less than a microsecond, in analogy to [76].

10. Quantum walks with non-orthogonal position states

10.1. Overview

In the theoretical description of QWs, it is almost universal practice to model the different "positions" by mutually orthogonal subspaces in Hilbert space. However, as we have seen in the previous sections, orthogonality cannot be achieved in some proposals [110, 124, 95] and the related experiments [101, 72, 125]. In order to fit these experiments to the theoretical model, it was necessary to choose the step size $|\Delta\alpha|$ sufficiently large to make these states approximately orthogonal.

In this section, which follows closely [71], we show that the lack of orthogonality can be exploited. Firstly, we give a complete analysis of quantum walks with non-orthogonal position states. In particular, we will introduce a transformation to the orthogonal case, such that all known results for that case can be utilized. As a result, it is no longer necessary to avoid the overlaps between different position states in experiments with trapped ions. Hence, in the experimental setup described in the previous sections, one can consider smaller step sizes and run the walk for more steps before the LDA (8.10) breaks down.

Secondly, the transformation of the nQW into a QW with orthogonal position states encodes the properties of the non-orthogonality into the initial state of the QW. Hence, by utilizing the overlap, it is possible to simulate QWs with interesting initial states, in particular those, which are extended over several positions, such as considered in [112]. In contrast to an experimental setup with orthogonal position states and a localized initial state, this simulation does not need an elaborate preparation process, which would require several additional operations, some of which must involve a breaking of the translational symmetry. Such a preparation process would severely decrease the fidelity of the experiment.

Furthermore, we show how the initial state can be shifted in momentum space by including an additional operation into the walk operator. This allows for the control of the scaling and the measurement of the dispersion relation, providing a benchmarking tool for the quantum walk. Finally, we use this method of momentum shifts to implement Bloch oscillations [35] as an example for the range of experiments with nQWs, which can be readily implemented using state-of-the-art technology.

Throughout this section, we relate our theory to the trapped-ion setting (cf. Fig. 8.1). However, it applies to arbitrary unitary nQWs in any dimension.

10.2. Transformation into an orthogonal QW

In the following, we will show that the nQW with a localized initial state is equivalent to an (orthogonal) QW, where the initial state is in a superposition of several position states.

For the basis $\{|\alpha_x\rangle\}$, there exists a dual basis $\{|\alpha'_x\rangle\}$, defined by $\langle\alpha_x|\alpha'_y\rangle = \delta_{xy}$ for all x, y. A relation is given by the Gram matrix Γ by $\{|\alpha'_x\rangle = \Gamma^{-1}|\alpha_x\rangle\}$ [24]. We can therefore define an orthonormal basis by $\{|e_x\rangle = \Gamma^{-1/2}|\alpha_x\rangle\}$ with $\Gamma^{-1/2}$ being hermitian. Since $[S, G] = 0$, the action of the shift operator in the orthonormal basis is given by

$$S|e_k\rangle \otimes |c_\pm\rangle = |e_{k\pm1}\rangle \otimes |c_\pm\rangle . \tag{10.1}$$

Therefore, the walk operator W also defines a QW in the orthonormal basis. The probability to find the walker in position $|e_x\rangle$ is given by the projector $\Gamma^{-1/2} F_x \Gamma^{-1/2}$, such that we can transform Eq. (8.3) to

$$P_t(x) = \mathrm{Tr}\Big(\big(|e_x\rangle\langle e_x| \otimes \mathbb{1}\big)\cdot W^t \widetilde{\rho}_0 W^{-t}\Big), \tag{10.2}$$

where the initial state amounts to

$$\widetilde{\rho}_0 = \frac{G\widehat{\rho}_0 G}{\mathrm{Tr}(G\widehat{\rho}_0 G)} \tag{10.3}$$

with $\widehat{\rho}_0 = |e_0\rangle\langle e_0| \otimes \rho_{00}$. Due to the overlap function (8.2), $\widetilde{\rho}_0$ is extended over several position states.

10.3. Fourier transformation and asymptotic behaviour

In this section, we investigate the properties of the nQW using Fourier methods and asymptotic perturbation theory [8, 45, 5]. The Fourier transform of the position space $\ell_2(\mathbb{Z})$ is the momentum space $L^2\big([-\pi,\pi)\big)$. With the coin space tensored to it, we consider the system in momentum space as $L^2\big([-\pi,\pi),\mathbb{C}^2\big) \cong L^2\big([-\pi,\pi)\big)\otimes\mathbb{C}^2$. That is, the Fourier transform of a vector

$$\psi = \sum_x |e_x\rangle \otimes |\psi_x\rangle \in \ell_2(\mathbb{Z}) \otimes \mathbb{C}^2 \tag{10.4}$$

is a $\mathbb{C}^2$-valued function of p, given by

$$\psi(p) = \sum_x e^{ip\cdot x}|\psi_x\rangle \in \mathbb{C}^2. \tag{10.5}$$

The walk operator W is translation invariant on $\ell_2(\mathbb{Z})$ and thus acts as a multiplication operator in momentum space, i.e. $\big(W\psi\big)(p) = W(p)\psi(p)$, with $W(p) = S(p)\cdot C$ and $S(p) = \exp(i\,p\,\sigma_z)$.

From the eigendecomposition

$$W(p) = \sum_{k=1}^{2} e^{i\omega_k(p)} P_k(p), \tag{10.6}$$

we obtain the dispersion relations $\omega_k(p)$ and the corresponding eigenvectors $\psi_k(p)$, with $P_k(p)$ denoting the projector on the subspace spanned by $\psi_k(p)$. The eigenvectors $\psi_k(p)$ define Bloch waves with distinct momentum p. The dispersion relations $\omega_k(p)$, i.e. the band structure, encode the fundamental transport properties of that system. Hence, it plays the same role as for a particle in a periodic potential, like an electron in a solid-state system. Indeed, the group velocities $v_k(p) = \mathrm{d}\omega_k(p)/\mathrm{d}p$ (cf. Fig. 10.1a) determine the spreading behaviour of the (initial) state of the QW. The ballistic order of the spreading, i.e. the one linear in t, can be captured by the asymptotic position-probability distribution $P_\infty(q)$, where $q \in [-1,1]$ denotes the asymptotic scaled ($\propto 1/t$) position variable. It was shown in [5] that $P_\infty(q)$ is the inverse Fourier transform of the characteristic function

$$C_{\widetilde{\rho_0}}(\lambda) = \int_{[-\pi,\pi)} \mathrm{d}p \; \mathrm{Tr}\left(\widetilde{\rho_0}\,(p) \cdot e^{i\lambda V(p)}\right), \tag{10.7}$$

where $V(p) = \sum_k v_k(p) P_k$ is the group-velocity operator and $\widetilde{\rho_0}(p) = |g(p)|^2 \rho_{00}$ the initial state with $g(p)$ being the Fourier transform of the overlap function $g(x)$. Therefore, the influence of the group velocities $v_k(p)$ on the asymptotic probability distribution is determined by $|g(p)|^2$, for each momentum p.

As shown in Fig. 10.1a, the group velocities of the cases C_E and C_H are the same, but shifted by $p = \pi/2$. Hence, we are able to explain why the experimental and Hadamard walk lead to the same probability distribution in the orthogonal case, but to different ones in the non-orthogonal case, as shown in Fig. 8.2: In the orthogonal case, $g(p)$ is constant in p. Hence, all velocities $v_k(p)$ occur with equal weight, leading to non-zero probabilities in the whole range $x \in \left[-t/\sqrt{2}, t/\sqrt{2}\right]$ (Fig. 8.2). The maximal velocities $v_k(p) = \pm 1/\sqrt{2}$ play a special role by the formation of caustics, leading to the well-known peaks at $x = \pm t/\sqrt{2}$ [5]. In the non-orthogonal case however, $g(p)$ is localized at $p = 0$, such that only the group velocities around $p = 0$ influence the nQW (Fig. 10.1a). In the Hadamard walk, $v_k(0) = \pm 1/\sqrt{2}$, i.e. the velocities that are also most pronounced in the orthogonal case, whereas in the experimental case $v_k(0) = 0$, such that the position probability remains at the initial position.

Due to the small but finite width of $g(p)$, also group velocities close to $p = 0$ influence the nQW. Since in the case C_E they change strongly around $p = 0$, the width of the peak in position space increases linearly in t (See [72] for numerical results). Similarly, also in the case C_H the widths of the two peaks in position space increase with t, but at a much smaller rate (Fig. 10.1b).

10.4. Controlling the spreading rate

In this section, we describe a method to shift the dispersion relation in momentum space and thus to change the spreading rate of the nQW. For a momentum shift of the amount of Θ, we apply after each step the operator $\mathbb{1} \otimes R(\Theta) = \mathbb{1} \otimes \exp(i\,\Theta\,\sigma_z)$. This is equivalent to a nQW with the effective walk operator

$$W_\Theta(p) = S(p + \Theta) \cdot C, \tag{10.8}$$

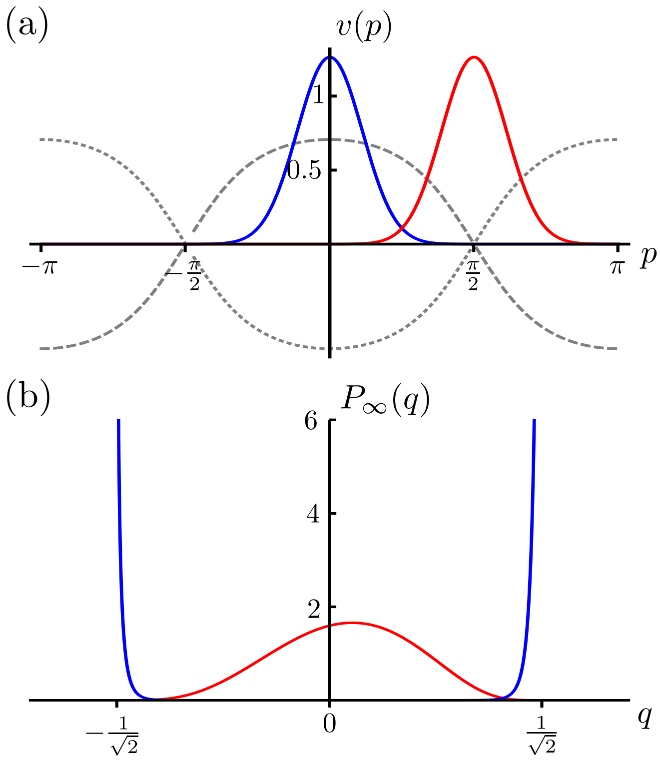

Figure 10.1.: (a): Group velocities $v_k(p)$ (grey, dotted/dashed) of the Hadamard walk and $\|\widetilde{\rho_0}\|(p)/(2\pi)$ of the initial states localized at $p = 0$ (blue) and $p = \pi/2$ (red, corresponds to the experimental walk) with $\sigma = 4$. (b): Asymptotic position-probability distribution $P_\infty(q)$ for each initial state (blue, red). For each initial state, only the group velocities around their points of localization determine the position-probability distribution. That is, since the blue initial state (a) is localized at $p = 0$, where $v_k(0) \approx \pm 1/\sqrt{2}$, $P_\infty(q)$ consists of two peaks moving away from the origin with that velocity (b). In contrast, the red initial state (a) is centered around $v_k(\pi/2) \approx 0$, which leads to a localized asymptotic position-probability distribution $P_\infty(q)$. The coin part of the initial states is $\rho_{00} = |c_+\rangle\langle c_+|$. Figure and caption from [71].

i.e. $R(\Theta)S(p) = S(p+\Theta)$, since $S(p) = \exp(i\,p\,\sigma_z)$. The time evolution is then determined by the group velocities $v_k(p+\Theta)$. Thus, using the experimental coin C_E, it is possible to achieve the spreading of a Hadamard walk by including the operator $R(-\pi/2)$ into W. In fact, since $C_H = \sigma_z C_E$, the momentum shift with $\Theta = -\pi/2$ compensates for the σ_z-factor, up to a complex phase.

Experimentally, the momentum shift provides a method for determining the dispersion relations $\omega_k(p)$ of a given walk operator W, if it is implemented in a non-orthogonal setting: Namely by performing a momentum-shifted nQW W_Θ for several values of $\Theta \in [-\pi, \pi]$ and determining the scaling of the position-probability distribution for each Θ. In particular, if an implementation of the walk operator W is influenced by experimental imperfections and the dispersion relations are therefore not exactly known, this may serve as an important probing or calibration tool.

10.5. Simulating Bloch oscillations with quantum walks

In semi-conductor superlattices, a static external electric field leads to a linear drift of the electron momentum and due to the periodic band structure to an oscillatory behaviour of the electrons, detectable by optical methods, which is called Bloch oscillations [36].

This effect can be simulated in QWs in the sense that the linear drift is implemented by a momentum shift of $\Delta\Theta$ in each step of the QW. This is achieved by applying the operator $R(t\cdot\Delta\Theta)$ (modulo 2π) at the t-th step, for every t. The Bloch oscillations are manifested as an oscillating behaviour of the position-probability distribution, due to changing group velocities at each step of the walk (cf. Fig. 10.1a), in contrast to a linear spreading with a constant group velocity (Fig. 10.2). Although this effect does not require the non-orthogonality of the position states, the simple shape of the position-probability distribution of a nQW (two distinct Gaussian peaks, cf. Fig. 8.2) can reduce the effort for detection. A different method for the implementation of Bloch oscillations was proposed in [92]. However, their method requires a position-dependent coin operator, which may need a higher technical effort.

As mentioned earlier, trapped ions provide a convenient system for nQWs. We showed that the demand for orthogonality can be relaxed and, indeed, for the implementation of Bloch oscillations a small step size $|\Delta\alpha|$ is favoured, which allows for a significantly higher number of steps within the LDA (8.10). Moreover, the proposed protocol for the shift operator via photon kicks, cf. Section 9, allows for an even higher number of steps. In Fig. 10.2, the oscillating probability distribution is shown for a possible choice of parameter values for a Lamb-Dicke parameter of $\eta \leq 0.31$, as in Ref. [72]. The momentum-shift operator $R(\Theta)$ can be implemented by shifting the phase of the driving light fields with respect to the relative phase of the coin states [50]. The positions of the peaks can be determined using state-of-the-art blue-sideband protocols [122].

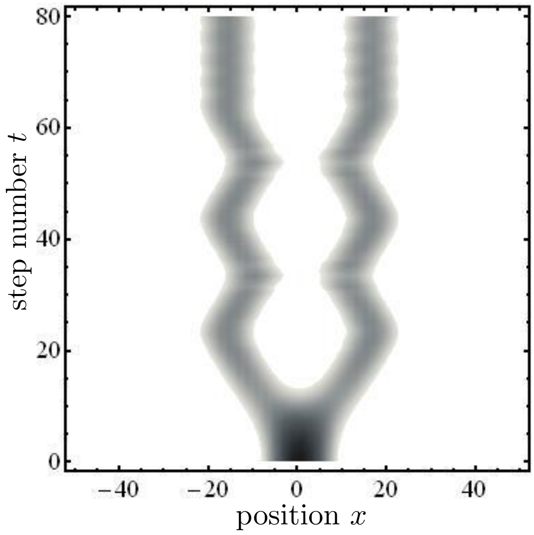

Figure 10.2.: Probability density (greyscale with black: $P_t(x) = 1$) of a Hadamard nQW ($\sigma = 14$) with Bloch oscillations. The nQW starts with 20 steps without momentum shift, such that two peaks separate from the origin with velocity $1/\sqrt{2}$ (cf. Fig. 8.2b). Then the Bloch oscillations are switched on with $\Delta\Theta = \pi/10$, such that the positions of the peaks oscillate with a period of 20 steps and an amplitude of 5 positions. The Bloch oscillations are switched off after 65 steps, a point where the group velocity is zero (cf. Fig. 10.1a), such that the peaks remain at their position during the remaining nQW. The expectation values of the harmonic-oscillator occupation-number operator N range during the oscillations from $\langle N_{min} \rangle = 1.3$ to $\langle N_{max} \rangle = 2.7$, which is detectable with state-of-the-art trapped-ion technology [122]. Figure and caption from [71].

10.6. Summary

We obtained an intuitive description of nQWs in terms of dispersion relations by transforming them into orthogonal QWs and applying asymptotic methods. Furthermore, we introduced the momentum-shift method, which allows for changing the spreading behaviour, determining the dispersion relation, and, by the correspondence to solid-state systems, for the implementation of the analog effect of Bloch oscillations. Hence, the non-orthogonality can be exploited and does not need to be avoided. In experiments with trapped ions, nQWs allow for a higher number of steps within the LDR, due to smaller step sizes, and a new range of experiments with available technology.

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Curriculum Vitae

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Studies

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Publications

1 H. Schmitz, A. Friedenauer, Ch. Schneider, R. Matjeschk, M. Enderlein, T. Huber, J. Glueckert, D. Porras, T. Schaetz. The “Arch” of Simulating Quantum Spin Systems with Trapped Ions. *Appl. Phys. B*, 95:195–203, 2009.

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