
Entanglement entropy in quantum many-particle systems and their simulation via ansatz states

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Zusammenfassung

Im Gegensatz zu klassischen Vielteilchensystemen, für welche die Anzahl der Freiheitsgrade linear mit der Systemgröße anwächst, wächst sie für quantenmechanische Vielteilchensysteme exponentiell an. Auf der einen Seite verspricht die resultierende Komplexität der Quantensysteme großes Potential bei direkter technischer Ausnutzung. So werden seit einigen Jahren zum Beispiel intensivst die Grundlagen für die Realisierung von Quantencomputern und deren Anwendungsmöglichkeiten erforscht. Auf der anderen Seite erschwert dieser hohe Komplexitätsgrad, besonders in Regimen starker Korrelationen, den Zugang zum Verständnis der physikalischen Prozesse in derartigen Systemen über analytische oder numerische Verfahren. So kommt es, dass einige technologisch hoch relevante Systeme wie die Hochtemperatursupraleiter bis zum heutigen Tage unzureichend verstanden sind.

Ein Hauptgegenstand dieser Arbeit besteht daher in der Entwicklung von effizienten numerischen Methoden für stark korrelierte quantenmechanische Gittersysteme. Für eindimensionale Systeme gibt es eine solche sehr erfolgreiche Methode, die Dichtematrixrenormierungsgruppe (DMRG). Das Charakteristikum dieser Methode ist, dass der physikalische Zustand über eine bestimmte Klasse von Ansatzzuständen möglichst gut approximiert wird, diese aber so konstruiert sind, dass das exponentielle Wachstum der Anzahl der Freiheitsgrade vermieden wird. Mittels DMRG können Grundzustände eindimensionaler wechselwirkender Vielteilchensysteme oft mit extrem hoher Präzision bestimmt werden. Dies deutet bereits darauf hin, dass Grundzustände die prinzipiell exponentiell wachsende Zahl von Freiheitsgraden oft gar nicht ausschöpfen, sondern über wesentlich weniger Parameter effizient beschrieben werden können. Die der DMRG zugrundeliegende Klasse von Ansatzwellenfunktionen sind die sogenannten Matrixproduktzustände. Bei der Wahl von entsprechenden geeigneten Ansatzwellenfunktionen für höhere Raumdimensionen, kommt es entscheidend darauf an, dass diese in der Lage sind, das Skalierungsverhalten der Quantennichtlokalität (z.B. über die Verschränkungsentropie quantifiziert) mit einer möglichst geringen Parameteranzahl richtig modellieren zu können.

Aus diesem Grunde wird im ersten Teil der Arbeit numerisch und analytisch untersucht, wie die Quantennichtlokalität in verschiedenen physikalisch relevanten Szenarien mit der Systemgröße oder der Zeit skaliert. Unter anderem wird das Skalierungsverhalten der Rényi-Entropien im Rahmen der 1+1-dimensionalen konformen Feldtheorie hergeleitet und die Abhängigkeit von den Randbedingungen bestimmt. Bestehende Vermutungen und analytische Hinweise zum Verhalten der Verschränkungsentropie in kritischen fermionischen und bosonischen Systemen werden numerisch mit hoher Präzision bestätigt. Für integrable Systeme werden allgemeine Bedingungen hergeleitet, unter denen ein System lokal in einen statischen Zustand konvergiert. Dieser ist nicht-thermisch und trägt In-

formationen über den Anfangszustand des Systems. Die Verschränkungsentropie ist für derartige statische Zustände extensiv. Für kurze Zeiten steigt die Verschränkungsentropie in der Regel linear in der Zeit an, was letztendlich in einem exponentiellen Wachstum des Rechenaufwands für die DMRG resultiert. Daraus folgt, dass zeitabhängigen DMRG-Simulationen der direkte Zugang zu langen Zeiten im Allgemeinen verwehrt ist.

Der zweite Teil der Arbeit fokussiert auf die Weiterentwicklung der erwähnten numerischen Verfahren. Zunächst wird die zeitabhängige DMRG mit einer allgemeinen Extrapolationsmethode für die während der Simulation bestimmten Observablen kombiniert. Auf diese Weise kann das Problem des Entropiewachstums umgangen und Spektralfunktionen mit hoher Präzision bestimmt werden. Das Verfahren wird am Beispiel des Heisenberg-Antiferromagneten im Vergleich mit Bethe-Ansatz-Daten für $T = 0$ und Quanten-Monte-Carlo-Daten für $T > 0$ demonstriert. Für die Simulationen von höherdimensionalen Systemen haben sich die Projected-Entangled Pair-States (PEPS) und Multi-scale Entanglement Renormalization Ansatzzustände (MERA) als geeignete Wellenfunktionsklassen erwiesen. Zunächst konnten diese ausschließlich für Spinsysteme verwendet werden. Im Rahmen der Doktorarbeit werden Varianten dieser Zustandsklassen für den fermionischen Fall vorgeschlagen und es wird eine Methode entwickelt, die es erlaubt, die bekannten Algorithmen für Spinsysteme auf den Fall von Fermionen zu übertragen. Dabei steigt der notwendige Rechenaufwand nur um einen vernachlässigbaren Overhead. Erste numerische Testanwendungen verliefen erfolgreich. Damit steht ein neues Verfahren zur Verfügung, mit dem nun z.B. das zweidimensionale Hubbard-Modell untersucht werden kann. Dieses Modell ist ein Kandidat für die Beschreibung der Physik in Hochtemperatursupraleitern.

Summary

In contrast to classical many-particle systems for which the number of degrees of freedom grows linearly with the system size, it grows exponentially for quantum many-particle systems. On the one hand, the resulting complexity of the quantum systems has a high potential for technological advances if it can be exploited directly. For example, in recent years, the fundamentals for the realization of quantum computers and their possible applications have been investigated intensely. On the other hand, the high complexity, especially in strongly correlated regimes, often makes the analytical or numerical analysis of underlying physical phenomena very difficult. This is why some systems of high technological relevance, like the high-temperature superconductors, are still unsatisfactorily understood.

A main topic of this thesis is the development of efficient numerical methods for the simulation of strongly correlated quantum lattice models. For one-dimensional systems, the density-matrix renormalization-group (DMRG) is such a very successful method. The physical states of interest are approximated within a certain class of ansatz states. These ansatz states are designed in a way that the number of degrees of freedom are prevented from growing exponentially. With the DMRG method, ground states of interacting one-dimensional systems can often be determined with very high precision. This observation indicates already that ground states actually do not exhaust the available exponential number of degrees of freedom but can be described efficiently with much fewer parameters. The ansatz states used in DMRG are the so-called matrix product states. A very useful criterion for the construction of corresponding appropriate ansatz states for higher-dimensional systems is the quantum nonlocality as for example quantified by the entanglement entropy. The ansatz states should be able to reproduce the scaling properties of the quantum nonlocality in the physical states of interest with as few parameters as possible.

The first part of the thesis, therefore, provides analytical and numerical analysis of the scaling of quantum nonlocality with the system size or time in different, physically relevant scenarios. For example, the scaling of Rényi entropies and their dependence on boundary conditions is derived within the 1+1-dimensional conformal field theory. Conjectures and analytical indications concerning the properties of entanglement entropy in critical fermionic and bosonic systems are confirmed numerically with high precision. For integrable models in the thermodynamic limit, general preconditions are derived under which subsystems converge to steady states. These steady states are non-thermal and retain information about the initial state. It is shown that the entanglement entropy in such steady states is extensive. For short times, the entanglement entropy grows typically linearly with time, causing an exponential increase in computation costs for the DMRG method. Consequently, time-dependent DMRG simulations usually have no direct access to the long time

regime.

The second part of the thesis focuses on the development and improvement of the above-mentioned numerical techniques. The time-dependent DMRG is complemented with an extrapolation technique for the evaluated observables. In this way, the problem of the entropy increase can be circumvented, allowing for a precise determination of spectral functions. The method is demonstrated using the example of the Heisenberg antiferromagnet and results are compared to Bethe-Ansatz data for $T = 0$ and quantum Monte Carlo data for $T > 0$. For the simulation of higher-dimensional systems, projected-entangled pair-states (PEPS) and the multiscale entanglement renormalization ansatz (MERA) turn out to be appropriate wavefunction classes. Initially, they could only be used for spin systems. Within this thesis, variants of those state classes are being suggested for the fermionic case. It is shown how the known algorithms for spin systems can be translated into corresponding algorithms for the fermionic systems. The occurring computation costs increase only by a marginal overhead. First numerical benchmarking tests proceeded successfully. Thus, new techniques are available which can for example be used to examine the two-dimensional Hubbard model. This model is a candidate for the description of high-temperature superconductivity.

1. Introduction and overview

This thesis is concerned with quantum many-particle lattice systems, i.e., fermions or bosons that hop from site to site of a lattice and interact with each other or, similarly, interacting spins that are localized on the sites of a lattice. The two major topics are:

1. An investigation of the scaling of entanglement entropy in ground states and time-evolved states – in particular the question of how subsystem entropies scale with the linear size of the subsystem and how they depend on the various other system parameters,
2. The development of appropriate ansatz states, which are of tensor-contraction type, and corresponding algorithms for the simulation of such systems with classical computers.

The two topics are intimately connected. Entanglement entropy is one of the most prominent and useful quantitative measures for quantum nonlocality. The “more quantum” a system really is in a certain parameter regime, the more degrees of freedom are involved. The maximum number of the degrees of freedom scales exponentially with the number N of lattice sites. Studying the entanglement entropy teaches us that systems of interest often do actually not exploit this seemingly insurmountable number of degrees of freedom. This allows us in some cases to approach such systems with analytical techniques or (at least) to simulate them on our classical computers. The second part of this thesis is focused on corresponding simulation algorithms that operate on different classes of what will be called *tensor contraction states*. A key issue here is the organization of the degrees of freedom of the corresponding class of ansatz states. It should reproduce the entanglement properties of the investigated systems appropriately. A deviation from this principle would result in numerical inefficiency or even complete failure of the simulation. The degrees of freedom in the ansatz state, in a sense, have to match the physical degrees of freedom that the considered quantum system actually exploits.

It is the goal of this work to provide substantial contributions to the field of many-particle quantum physics. In particular, analytical and numerical investigations are conducted providing new insights on the scaling of the entanglement entropy in ground states and time-evolving states, and new practical simulation techniques are developed based on tensor contraction states.

1.1. Challenge in the analysis of quantum many-particle systems

The fundamental difficulty in the analysis of quantum many-body (lattice) systems is due to the large size of the Hilbert space. Given a lattice $\mathcal{L}$ consisting of N sites, and associated with each site $x \in \mathcal{L}$, a local Hilbert space $\mathcal{H}_x$ of dimension d , the total Hilbert space $\mathcal{H} = \bigotimes_x \mathcal{H}_x$ has dimension

$$\dim(\bigotimes_{x \in \mathcal{L}} \mathcal{H}_x) = d^N, \quad (1.1)$$

i.e., the dimension scales exponentially in the number of lattice sites. In contrast to classical many-body systems where the number of degrees of freedom increases linearly with the system size, it increases exponentially for quantum systems. This mathematical property corresponds to the fact that quantum systems are “nonlocal”. For classical systems the state of the full system can be specified by specifying the states of all subsystems, e.g., for each lattice site the number of particles and/or the spin orientation. For a quantum system in a pure state $|\psi\rangle \in \mathcal{H}$, however, it is in general not sufficient to specify the reduced density matrices $\hat{\rho}_x = \text{Tr}_{\mathcal{L} \setminus \{x\}} |\psi\rangle\langle\psi|$ for all sites x . The state $|\psi\rangle$ contains more information than the collection of subsystem density matrices, in particular information about correlations of the subsystems. In comparison to classical systems, the nonlocality makes quantum systems much more complex but also more powerful – a notion that can be substantiated in the following sense:

If, on the one hand, we had a scalable quantum computer [1], which is a computing device that exploits quantum nonlocality, several tasks like factoring [2, 3] or searching in an unsorted database [4, 5] could be executed faster than with any known algorithm on classical computers. Conversely, the quantum computer can of course execute any classical program with the same number of operations as the classical computer.

On the other hand, quantum systems are harder to analyze. What precisely “harder” means is a topic of complexity theory. Following earlier works [6, 7], it was for example shown in Ref. [8] that the *2-local Hamiltonian* problem is *QMA-complete*: The *k-local Hamiltonian problem* concerns Hamiltonians on N qubits (spins 1/2) which contain only interaction terms acting on at most k , not necessarily neighboring, qubits. The problem poses the question whether the ground state energy of such a Hamiltonian is below some energy E or above $E + \Delta E$ with some finite (small) ΔE . The complexity class Quantum Merlin Arthur (*QMA*), introduced in Refs. [9, 6], is the quantum analog of the classical complexity class *NP*; see footnote ¹ for short definitions. For the complexity classes P ,

¹ The complexity classes that are referred to here concern *decision problems*, i.e., questions on an infinite set of inputs, e.g., given as bit strings, that have answers ‘yes’ or ‘no’, corresponding to a single output bit. The specification of solutions to many practically relevant tasks such as the traveling salesman problem, where the answer is a route, require more than one bit. Such tasks are called *function problems*. As long as the number of output bits scales polynomially in the number of input bits, such problems can be mapped to a collection of decision problems and the results on the corresponding complexity classes translate trivially.

P is the class of decision problems that can be solved in polynomial time on a classical computer,

NP , and QMA , the following inclusion relations hold:

$$P \subseteq NP \subseteq QMA, \quad (1.2)$$

and it is generally believed that the classes are distinct; the converse would have earth-shattering consequences. A problem is called *hard* for a given complexity class, if all other problems of that class can be mapped to it with, at most, a polynomial loss in computation efficiency. The problem is called *complete*, if it is hard and itself inside the class.

So the result of Ref. [8] implies that the problem of finding the ground state energy of *arbitrary* 2-local Hamiltonians is already among the hardest problems in QMA . Hence, it is potentially even too complex for a quantum computer to solve in polynomial time: QMA is the quantum analog of NP ; the quantum analog of P would be BQP , which is the class of decision problems solvable by a quantum computer in polynomial time, with an error probability of at most $1/3$. In an effort to restrict the class of considered Hamiltonians to physically more relevant settings, the result of Refs. [6, 8] has been extended to the 2-local Hamiltonian problem restricted to nearest-neighbor interactions on a two-dimensional (2D) square qubit lattice [10], or even translationally invariant nearest-neighbor interactions on a one-dimensional (1D) lattice [11].

In comparison to the discussed problem of finding the ground state energy for quantum systems, the task of finding the ground state energy of *classical* k -local Hamiltonians is equivalent to the so-called $MAX-k$ -SAT problem. $MAX-2$ -SAT is NP -complete, even under restriction to geometrically local interaction terms in two-dimensional real-space. So, quantum local Hamiltonian problems are harder to solve than classical ones, if $QMA \neq NP$.

1.2. Techniques for the analysis of quantum many-particle systems

The astonishing results presented in the previous section do however not imply that determining ground state properties of a particular (physical) system is in general a hopeless endeavor. Complexity theorists rather prove that certain classes of Hamiltonians contain representatives for which ground state properties are hard to obtain. The Hamiltonians that are constructed to prove the hardness of the ground state energy decision problems are still relatively artificial and, in particular not translationally invariant [10], or work with local Hilbert spaces of relatively large dimension [11].

meaning that the number of operations scales polynomially with the number of input bits.

NP is the set of all decision problems where for each 'yes'-case, there exists a proof for the fact that the answer is really 'yes' that can be verified in polynomial time by a deterministic Turing machine (a classical computer) – or, equivalently, the set of decision problems solvable in polynomial time by a non-deterministic Turing machine. NP contains for example the traveling salesman problem.

QMA is the set of decision problems where for each 'yes'-case, there exists a polynomial-size quantum proof (a quantum state for a polynomial number of qubits) which convinces a polynomial-time quantum verifier (a program on a quantum computer that finishes in polynomial time, e.g., a quantum circuit with a polynomial number of gates) with high probability of the fact that the answer is really 'yes'. Also, when the answer is 'no', every polynomial-size quantum state is rejected by the verifier with high probability.

The technical challenges posed by quantum nonlocality and the general complexity of determining ground state properties, or good approximations thereof, can be approached in different ways. Several of the most successful analytical and numerical techniques are summarized in the following and it is stressed what approximations are used to reduce the complexity of the problem. This will also motivate the need for the numerical methods addressed in this thesis and put them into context. In particular, the theoretical understanding of strongly correlated two-dimensional fermionic or frustrated spin systems is still incomplete and the development of new techniques for those cases is of great interest as discussed below in Sec. 1.3.

Exact diagonalization

The Hamiltonians of systems below a certain size can be *diagonalized exactly*. One can treat larger systems by not determining all eigenstates but only the ground state [12, 13] by Krylov subspace methods as for example the Lanczos algorithm [14], and by exploiting symmetries. Similar techniques can be used to obtain time-evolved states [15, 16]. For the $S^z = 0$ sector of translation invariant spin 1/2 models one can nowadays treat systems of around 40 sites.

Exact diagonalization of quasi-free systems and Bethe ansatz integrable systems

The complexity of the problem is reduced drastically for *quasi-free* and *Bethe ansatz integrable* systems [17–20]. Quasi-free systems, Hamiltonians which are quadratic forms in annihilation and creation operators, can be diagonalized by solving a single-particle eigenstate equation. The ground states and thermal states are Gaussian states, i.e., fully characterized by the single-particle Green's functions $\langle a_i a_j^\dagger \rangle$ and $\langle a_i a_j \rangle$. Hence, there are at most $\mathcal{O}(N^2)$ degrees of freedom.

Certain models of interacting one-dimensional lattice systems can be solved by the Bethe ansatz. Here, the many-particle physics is reduced not to single-particle but to two-particle physics, in the sense that the many-particle scattering matrices are two-body reducible [21, 18], i.e., that they can be expressed as products of two-body scattering matrices. For example, the ground state is determined by solving a system of M coupled equations for M rapidities, for example with $M = N/2$ for the $S^z = 0$ sector of a spin model.

Mean-field theory

Mean-field approaches reduce the problem with interaction, in an approximation, to a quasi-free one. The interactions with other particles are accounted for by introducing a (self-consistent) extra term in the single-particle Hamiltonian. In the case of a density-density interaction, the extra term could for example be the density operator coupled to a scalar (mean) field that represents the density of the other particles. The single-particle

problem is then solved self-consistently with respect to the mean field. The resulting many-particle state is a tensor product of the single-particle states, showing the severity of the approximation. It should be valid for phases where correlations between the particles and the fluctuations of the order parameter around its mean-field value are small. The mean-field approach can be formulated rigorously in the path integral picture as a Hubbard-Stratonovich transformation, introducing a new auxiliary field, followed by a saddle-point approximation with respect to the auxiliary field.

Density functional theory

The situation is quite similar in *density functional theory* [22–25], where the Kohn-Sham equations, which are again single-particle equations, have to be solved self-consistently with respect to the electron density. The approximation applied here concerns the exchange-correlation energy functional which is actually nonlocal but usually approximated to be local, e.g., in the *local density approximation* or *generalized gradient approximation*.

Dynamical mean-field theory

Dynamical mean-field theory (DMFT) [26–29] goes beyond the mean-field approximations. The interacting lattice problem is reduced to a self-consistent impurity problem where particles interact only on a single site: Using the so-called cavity method, one derives from the action of the full lattice model an effective action S_{eff}^0 for a single site. This effective action is drastically simplified by considering the limit of an infinite lattice coordination or, equivalently, infinite space dimension. Taking this limit as an approximation, S_{eff}^0 becomes a function of the single-particle Matsubara Green's function $\mathcal{G}_0(\tau)$; terms with higher-order Green's functions vanish. This Green's function $\mathcal{G}_0(\tau)$ takes the role of the mean-field and has to be determined self-consistently. Therefore, this approach is referred to as "dynamical" mean-field theory, as $\mathcal{G}_0(\tau)$ encodes temporal correlations. The approximation neglects higher-order nonlocal fluctuations. In order to calculate the onsite Green's function from a given effective action S_{eff}^0 , one can apply a mapping to an equivalent impurity problem, mentioned above. This is still a many-particle problem, but a simpler one. In many cases it can be tackled numerically by exact diagonalization (restricting the size of the non-interacting bath), quantum Monte Carlo, numerical renormalization group, density-matrix renormalization group (see below), and several other methods.

Perturbation theory

In *perturbative approaches*, the Hamiltonian is split into an exactly solvable part $\hat{H}_0$ and the rest $\lambda\hat{V}$, the perturbation, i.e., $\hat{H} = \hat{H}_0 + \lambda\hat{V}$. Observables are then expanded as power series in the perturbation and estimates for them are obtained by evaluation of sums or integrals for truncated versions of the series²:

²The perturbative expansions often have convergence radius zero and are rather asymptotic series, meaning that the infinite series is divergent but an optimal truncation order of the series exists which yields the best

The *linked-cluster expansion* technique [30–33] is based on the Rayleigh-Schrödinger perturbation theory and is applicable if the ground state of the unperturbed Hamiltonian $\hat{H}_0$ is a product state with respect to real-space. The perturbative series can then be organized as sums of terms that act on small real-space clusters for which the necessary maximum cluster size increases with the truncation order of the expansion. This reduces the problem to a perturbation theory on small clusters, and enables efficient numerical calculations.

A predominantly analytical approach is the *diagrammatic perturbation theory* where $\hat{H}_0$ contains only single-particle terms and the many particle path integral is expanded in the perturbation. This leads via Wick’s theorem to series expressions for observables as sums and integrals over products of unperturbed single-particle Green’s functions and vertex functions of the interaction $\hat{V}$. The terms can be visualized in the form of *Feynman diagrams*. An alternative operator based derivation is commonly known as the *S-matrix expansion*. In certain physical situations, one can identify subclasses of diagrams that dominate (in certain limits) all other diagrams of the same order and allow for an exact summation of the perturbation series for that dominating diagram subclass, as for example in the random phase or non-crossing approximations.

Functional renormalization group

Perturbative approaches are restricted to weak interactions. But even for weak interactions, they are often plagued by infrared divergences when there is more than one energy scale in the problem. To solve this, one can supplement the diagrammatic perturbation theory with a renormalization group (RG) procedure [34–37] which treats the energy scales successively, as in the *functional RG* techniques [38–42]. One introduces an infrared cutoff Λ in the free single-particle Green’s function g (the propagator), resulting in a Λ -dependence of all vertex functions³. Differentiating with respect to Λ yields an exact hierarchy of differential equations for the vertex functions. By integrating the full infinite set of differential equations from a cutoff value Λ_0 with the trivial propagator $g^{\Lambda_0} = 0$ to a value $\Lambda_1 < \Lambda_0$, such that $g^{\Lambda_1} = g$, one would obtain the exact vertex functions of the interacting system. In the cases of interest, this is typically not possible and the approximation consists in truncating the hierarchy of differential equations at a certain order. In this way, the complexity of the problem has been reduced to an integration of a coupled system of differential equations for a set of momentum and frequency dependent vertex functions.⁴ The latter dependencies pose the largest remaining technical complication. The approximation used

approximation to the exact result (for the observable).

³The *k-particle vertex function* is the sum of all one-particle irreducible diagrams with k amputated incoming and k amputated outgoing lines (open indices at interaction vertices). Diagrams are called “one-particle irreducible” if they stay connected when a single propagator line is cut. The 1-particle vertex function is the self-energy. From the vertex functions one can for instance obtain all Green’s functions.

⁴The scheme introduced in Refs. [41, 43] focuses on vertex functions, i.e., derives the RG equations for vertex functions from the *effective action*. Alternative schemes derive RG equations for amputated connected Green’s functions from the *effective interaction* [40] or for other related k -particle functions from the *Wick ordered interaction* [42]. Truncating those different exact hierarchies of differential equations corresponds to slightly different approximations.

here differs profoundly from the one in the one-step perturbation theory and the method is not necessarily restricted to weak interactions. The criterion is that the truncation of the hierarchy needs to be valid along the full path of the renormalization procedure.

Quantum Monte Carlo

Numerical approaches to many-particle quantum systems have become more and more important. A prominent class are sampling techniques. Two of the earliest examples are the *variational Monte Carlo* (VMC) and the *diffusion Monte Carlo* (DMC) [44–47]. In VMC, an ansatz is made for the many-particle wavefunction, e.g., a Jastrow-type wavefunction [48]. The parameters of the trial wavefunction are optimized by minimizing the energy expectation value. For this purpose, the energy can be evaluated by sampling. In DMC, a trial wavefunction is evolved in imaginary time, corresponding in the infinite time limit to a projection onto the ground state. The time integrals for the corresponding propagators are evaluated by sampling. There are several *quantum Monte Carlo* (QMC) techniques that work at finite temperature and are especially suited for examinations of lattice models. All those schemes work by expressing expectation values in the form

$$\langle \hat{A} \rangle \equiv \text{Tr } \hat{\rho} \hat{A} = \sum_c p(c) A(c) \quad (1.3)$$

and Monte Carlo sampling occurs with respect to the configurations c . The way in which such a representation is achieved, is specific for the different methods. In the method of the seminal Ref. [49], also called *world line Monte Carlo*, the Hamiltonian is split into $p = \mathcal{O}(1)$ easily diagonalizable parts $\hat{H} = \sum_{i=1}^p \hat{H}_i$ and the thermal density matrix is then expanded using a Suzuki-Trotter decomposition, e.g., $e^{-\beta \hat{H}} = (\prod_{i=1}^p e^{-\Delta\tau \hat{H}_i})^M + \mathcal{O}(\Delta\tau^2)$, with $\Delta\tau = \beta/M$. Inserting suitable completeness relations between the exponential factors in this expansion, expectation values of observables that are diagonal in the chosen basis are of the form (1.3) and can be evaluated by sampling over the pM sets of basis states.⁵ The described method requires extrapolation in the imaginary time step $\Delta\tau$. Alternative expansion schemes avoid this. One is the *stochastic series expansion* [50] which is basically a high-temperature series expansion of the partition function and observables.⁶

⁵The typical situation for the splitting of the Hamiltonian is that each $\hat{H}_i = \sum_b \hat{H}_{i,b}$ is a sum of short-ranged interaction terms with disjoint spatial support. Each exponential factor can hence be written as a product of commuting local terms $e^{-\Delta\tau \hat{H}_i} = U_i = \prod_b U_{i,b}$ and matrix elements can be conveniently evaluated with respect to an orthonormal product basis $|\sigma\rangle = |\sigma_1 \dots \sigma_N\rangle$. The expectation value for an observable $\hat{A}$ that is diagonal in this basis attains the form $Z\langle\hat{A}\rangle = \lim_{M \rightarrow \infty} \sum_{\sigma_1 \dots \sigma_{pM}} \langle\sigma_1|U_1|\sigma_2\rangle \langle\sigma_2|U_2|\sigma_3\rangle \dots \langle\sigma_{p+1}|U_1|\sigma_{p+2}\rangle \dots \langle\sigma_{pM}|U_p|\sigma_1\rangle \langle\sigma_1|\hat{A}|\sigma_1\rangle$, where Z is the partition function. $Z = Z\langle\mathbb{1}\rangle$ and $Z\langle\hat{A}\rangle$ are of the desired form $\sum_c p(c)A(c)$, where $c = \bigoplus_{n=1}^{pM} \sigma_n$ and $A(c) = 1$ or $\langle\sigma_1|\hat{A}|\sigma_1\rangle$, respectively.

⁶The Hamiltonian is a sum of bond terms $\hat{H} = \sum_b \hat{H}_b$. Following a Taylor expansion of the observables in the inverse temperature β , one arrives at the form $Z\langle\hat{A}\rangle = \sum_{\sigma} \sum_{N=0}^{\infty} \sum_{b_1, \dots, b_N} \frac{(-\beta)^N}{N!} \langle\sigma|\prod_{n=1}^N \hat{H}_{b_n}|\sigma\rangle \langle\sigma|\hat{A}|\sigma\rangle$, which can be evaluated by sampling over the choice of bonds $b_1, \dots, b_N$ and basis states $|\sigma\rangle$. For a Hamiltonian with N_b identical bond interaction terms $\hat{H}_b$, the average expansion order is roughly $\bar{N} \sim \beta N_b \langle\hat{H}_b\rangle$ and the variance typically scales as $(N - \bar{N})^2 \sim \bar{N}$ [50, 51].

The second alternative is the *path integral formulation* of QMC [52], where one starts from the many-body path integral and a splitting of the Hamiltonian into a part $\hat{H}_0$ that is diagonal in a basis of real-space product states and the rest $\hat{V}$. As in the diagrammatic perturbation theory, the path integral is expanded in $\hat{V}$. Sampling occurs over the terms in $\hat{V}$, the set of basis states, and for the evaluation of the imaginary-time integrals. Yet another variant of QMC departs from the fixation on real-space. In the *diagrammatic Monte Carlo* [53], the many-body path integral is expanded (with a different splitting of the Hamiltonian) just as in diagrammatic perturbation theory and sampling occurs, e.g., over Feynman diagrams. The method is, however, restricted to cases where the perturbation series is actually convergent and not of asymptotic character.

In the Monte Carlo schemes, the complexity of the many particle problem is reflected in the necessary sampling time to obtain observables to a given degree of accuracy. Initially, transitions between different configurations c during the sampling were done by local changes. Due to this, autocorrelation times for the observables, and hence the necessary simulation times, diverged at second order phase transitions. This was solved by introducing loop and worm algorithms for the configuration updates [54, 55, 51]. They are equivalents of the cluster updates [56] in classical Monte Carlo. Still, the computational cost grows with the amount of quantum correlations. To obtain ground state properties with the stochastic series expansion or path integral representation in the vicinity of a continuous quantum phase transition,⁷ one needs to scale the temperature for the simulation with the energy gap, resulting in a divergent average expansion order. The efficiency of the Monte Carlo schemes also relies on the condition that the function $p(c)$ in Eq. (1.3) can be treated as a probability distribution, i.e., is non-negative. For several frustrated spin models, and quite generically for fermionic models, this has not been achieved. In such cases, the simulation cost scales exponentially in the system size and the inverse temperature. This is known as the so-called *sign problem* of QMC [62, 63].

Numerical renormalization group

A purely numerical RG scheme for impurity problems (a small interacting system coupled to a bath of free particles), as occurring in the DMFT calculations described above, is the *numerical renormalization group* (NRG) technique [37, 64]. The energy band of the bath is split into a logarithmic set of intervals $|\varepsilon| \in [\Lambda^{-(n+1)}, \Lambda^{-n})$. The first approximation used in this method is to retain only one bath mode for each interval. The resulting dis-

⁷ Continuous phase transitions can occur when an external control parameter g is varied. They are accompanied by the onset of an order parameter at the critical point $g = g_c$ and a divergence of the correlation length in its proximity. In classical systems at finite temperature, the transitions are driven by the competition between the energy of the system and the entropy of its thermal fluctuations. In quantum systems, phase transitions are also possible at zero temperature, when a non-thermal parameter is varied [57, 58]. At the quantum critical point, the order is destroyed solely by quantum fluctuations. The spatial order parameter fluctuations become long-ranged and the energy gap to the first excited state vanishes. (That the gap necessarily vanishes when the correlation length diverges can be proven by application of Lieb-Robinson bounds [59–61].) Due to scale-invariance, observables depend via power laws on the system parameters, characterized by so-called critical exponents.

cretized model is mapped to a model on a semi-infinite chain by tridiagonalization of the impurity-bath coupling. The first site of the chain corresponds to the impurity system, the remaining sites to the bath degrees of freedom at lower and lower energy scales. This is the starting point for the RG scheme: Starting from the Hamiltonian restricted to the first few sites, in each step, the restricted Hamiltonian is diagonalized and the resulting eigenbasis is truncated to a finite number of states to retain only the low-energy subspace. Then another site is added, and the Hamiltonian for the enlarged system, projected to the reduced basis, is again diagonalized. In this way, the ground state can be determined by iterative diagonalization, accompanied with a truncation of high energy degrees of freedom. The computation cost scales cubically in the number of retained energy eigenstates.

Density-matrix renormalization-group

The *density-matrix renormalization-group* (DMRG) method was developed in a similar spirit [65, 66]. The objective is to calculate the ground state for a one-dimensional lattice system numerically. The method borrows the idea from NRG to work in an optimally chosen reduced basis. The (finite) system is split into three parts, a small central part for which the full basis is used and the left and right parts for which truncated sets of, say χ , basis states are retained. In each step of the simulation, the Hamiltonian of the full system is projected to the reduced Hilbert space for such a splitting of the system and the ground state $|\psi\rangle$ of the projected Hamiltonian is determined, e.g., by using the Lanczos algorithm [14]. Then one changes the choice for the splitting of the system and moves the central part for instance one site to the right, i.e., shifts one site from the central to the left part and one from the right to the central part. In doing so, the (reduced) basis of the left part is enlarged by a factor of d , which is the Hilbert space dimension for a single site. The RG-like feature consists now in retaining only χ of those $d\chi$ basis states for the left part. The applied criterion for the selection of states is not the energy, as in NRG, but the states are chosen as eigenstates of $\hat{\rho}_L = \text{Tr}_{C,R} |\psi\rangle\langle\psi|$, where $\text{Tr}_{C,R}$ denotes the trace over the central and the right part of the system. One retains the χ eigenstates of $\hat{\rho}_L$ that have the largest eigenvalues. This corresponds to keeping the most important summands in the Schmidt decomposition [67] of $|\psi\rangle$; see, e.g., [68, 69]. One continues now and sweeps forth and back through the system, optimizing the retained basis states more and more to obtain a better and better approximation to the real ground state. The computation cost and (ultimately) achievable accuracy of the approximation are determined by the number χ of retained basis states. Once the ground state is converged, observables can be evaluated easily. Variants of this method can be used to calculate for example spectral functions [70–72], time-evolved states [73–76], and to address systems at finite temperature [77–79] or in the thermodynamic limit [80, 81].

As it turns out, DMRG is not necessarily to be understood as a renormalization technique, but can, equivalent to the description above, be formulated as a variational method on a certain class of ansatz states [82] (see, e.g., also [68, 69]), the so-called *matrix product states* (MPS) [83–85]. All DMRG methods have in common that the manipulated

many-particle states are always of MPS form

$$|\psi\rangle = \sum_{\sigma_1, \dots, \sigma_N} \text{Tr}(A_1^{\sigma_1} A_2^{\sigma_2} \cdots A_N^{\sigma_N}) |\sigma_1 \sigma_2 \dots \sigma_N\rangle, \quad (1.4)$$

where $(|\sigma_i\rangle)_{\sigma_i = 1, \dots, d}$ are basis states of the Hilbert space of site i and the $A_i^{\sigma_i}$ are matrices (of size $\chi \times \chi$). The ground state algorithm, e.g., as described above in the traditional interpretation of DMRG, corresponds to an iterative variational optimization of the energy functional $E(\psi) = \langle \psi | \hat{H} | \psi \rangle / \langle \psi | \psi \rangle$. In each step of the iteration, the matrices for a small (central) subsystem are optimized, while all other matrices are kept fixed.⁸ One continues with the optimization of a neighboring site and sweeps forth and back through the lattice until the energy converges. In many examples of interacting systems, DMRG has been used to determine ground state properties correctly up to machine precision. In other DMRG algorithms, e.g., real- or imaginary-time evolution operators are applied to an MPS. Applying an evolution operator for a small time step to ψ exactly, requires in general an increase in the matrix size $\chi \rightarrow \chi' > \chi$. Due to limited computational resources, one can not let the matrix size increase further and further. So, after each time step, the matrix size is decreased by an optimal truncation procedure. It employs a Schmidt decomposition of the state. The computation cost is polynomial in the matrix size χ . It scales for example as χ^3 in the ground state and time-evolution algorithms for systems with open boundary conditions; see Sec. 1.5 for further details.

1.3. Potential of tensor contraction states for the description of 2D systems

The MPS in Eq. (1.4) is the prototype for the sort of ansatz states considered in the following: When expanding the many-body state in basis states $|\sigma_1 \dots \sigma_N\rangle$ that are tensor products of site basis states $\{|\sigma_i\rangle_{\sigma_i = 1, \dots, d}\}$, one generally obtains an exponential number of expansion coefficients $\psi_{\sigma_1 \dots \sigma_N}$, i.e., $|\psi\rangle = \sum_{\sigma} \psi_{\sigma} |\sigma\rangle$. For the ansatz states considered here, one reduces the number of degrees of freedom and expresses the expansion coefficients in the form of partially contracted sets of tensors. Therefore, they will be

⁸Let the central subsystem consist of (usually two) sites $i, i+1, \dots, j$, and let us define $B^{\sigma_i \dots \sigma_j} := A_i^{\sigma_i} A_{i+1}^{\sigma_{i+1}} \cdots A_j^{\sigma_j}$. Taking the derivative of the energy functional $E(\psi)$ with respect to $B := (B^{\sigma_i \dots \sigma_j} | \dots)$, one obtains an effective eigenvalue equation for it that can be solved with the Lanczos method [14]. After doing so we want to move, e.g., to the right, to optimize the degrees of freedom for the correspondingly shifted central system. Hence, one needs a transformation such that $B^{\sigma_i \dots \sigma_j} A_{j+1}^{\sigma_{j+1}} \approx \tilde{A}_i^{\sigma_i} \tilde{B}^{\sigma_{i+1} \dots \sigma_{j+1}}$ holds in a controllable approximation. This can be achieved by a singular value decomposition $B^{\sigma_i \dots \sigma_j} = C_i^{\sigma_i} \Lambda D^{\sigma_{i+1} \dots \sigma_j}$, where Λ is the diagonal matrix of singular values. This corresponds to the Schmidt decomposition of $|\psi\rangle = \sum_m \lambda_m |\ell_m\rangle \otimes |r_m\rangle$ and the singular values λ_m are the square roots of the eigenvalues of the reduced density matrix $\hat{\rho}_L = \sum_m \lambda_m^2 |\psi_m\rangle \langle \psi_m|$. The number of nonzero singular values is now in general larger than the original χ and therefore, needs to be truncated to retain only the largest χ , or some other number, corresponding to a suitable precision criterion. With the corresponding (diagonal) projection matrix P , the algorithm proceeds to the next iteration step with $\tilde{A}_i^{\sigma_i} = C_i^{\sigma_i} P$ and $\tilde{B}^{\sigma_{i+1} \dots \sigma_{j+1}} = P \Lambda D^{\sigma_{i+1} \dots \sigma_j} A_{j+1}^{\sigma_{j+1}}$. See, e.g., [69] for more details on the relation between the traditional and the MPS interpretation of DMRG.

called *tensor contraction states*, see Fig. 1.1. For MPS (1.4), those tensors are simply the matrices $A_i^{\sigma_i}$ and the partial contractions are matrix products. The structure of a decomposition of ψ_σ into a product of tensors is to be chosen such that the number of degrees of freedom (tensor elements) scales only polynomially with the system size N and such that an efficient optimization algorithm for the tensor elements can be devised. As pointed out before, the scaling of entanglement entropy can be used as a guiding principle for constructing such ansatz states. For this purpose, the next section summarizes results about the scaling of entanglement entropy in physically relevant scenarios.

With the existing analytical and numerical techniques, described in the previous section, weakly interacting regimes are typically well covered. For larger spatial dimensions $\gtrsim 3$, mean field approaches often work astonishingly well (for each model there exists an upper critical dimension above which mean field theory yields the correct critical exponents). For interacting electrons in three dimensions, e.g., the validity of the Fermi-liquid description⁹ is well accepted. Furthermore, strongly interacting one-dimensional lattice systems are for instance very well covered by DMRG and QMC. Regarding the long-wavelength properties, also the Luttinger liquid description¹⁰ is often a very good approximation. Also functional RG may yield an, at least qualitative, understanding. The situation is different for (strongly) interacting two-dimensional models. Except for certain limits, the Fermi liquid theory is not applicable and a controlled functional RG is already hard to implement. QMC works very well in several interesting cases, but it is inefficient for fermionic and frustrated magnetic models where the sign problem [62, 63] occurs. DMRG is essentially a technique for one-dimensional systems and inefficient for two dimensions. The reasons for this inefficiency will be explained in Sec. 1.5. Hence, there are several interesting two-dimensional (or effectively two-dimensional) systems which are still unsatisfactorily understood. A prominent example are high-temperature superconductors [91–93]. The Fermi-Hubbard model is a candidate for the description of the physics of the copper-oxide planes, typical for those superconductors. With the different types of tensor contraction states described above and the corresponding optimization algorithms, as addressed in this thesis, one attempts to fill that gap in the analytical and numerical description of two-dimensional models.

⁹The Fermi liquid theory describes the properties of “normal” metals. It was first introduced on a phenomenological basis by Landau. It relies on an one-to-one correspondence between the low-energy excitations of the free Fermi gas and those of the interacting electron system which are termed *quasiparticles*. They can be envisaged as particles whose motion is disturbed by the surrounding particles and which themselves perturb the particles in their vicinity. Remaining weak interactions between the quasiparticles lead to finite life times and scattering that can be described by a Boltzmann equation. The theory was substantiated by a microscopic perturbative derivation [86, 87], where the one-particle propagator and the two-particle vertex function are the key quantities, and also by renormalization group calculations.

¹⁰In one dimension, the Fermi liquid theory is not applicable since the low energy regime is dominated by collective excitations. In particular, the single particle Green’s function for a fixed momentum, as calculated in second order perturbation theory, does not feature a single quasiparticle pole. Luttinger liquid theory [88–90] focuses on the physics around the two Fermi points. The system can be mapped to a bosonic quasi-free model which, then, reflects already the separation of spin and charge degrees of freedom.

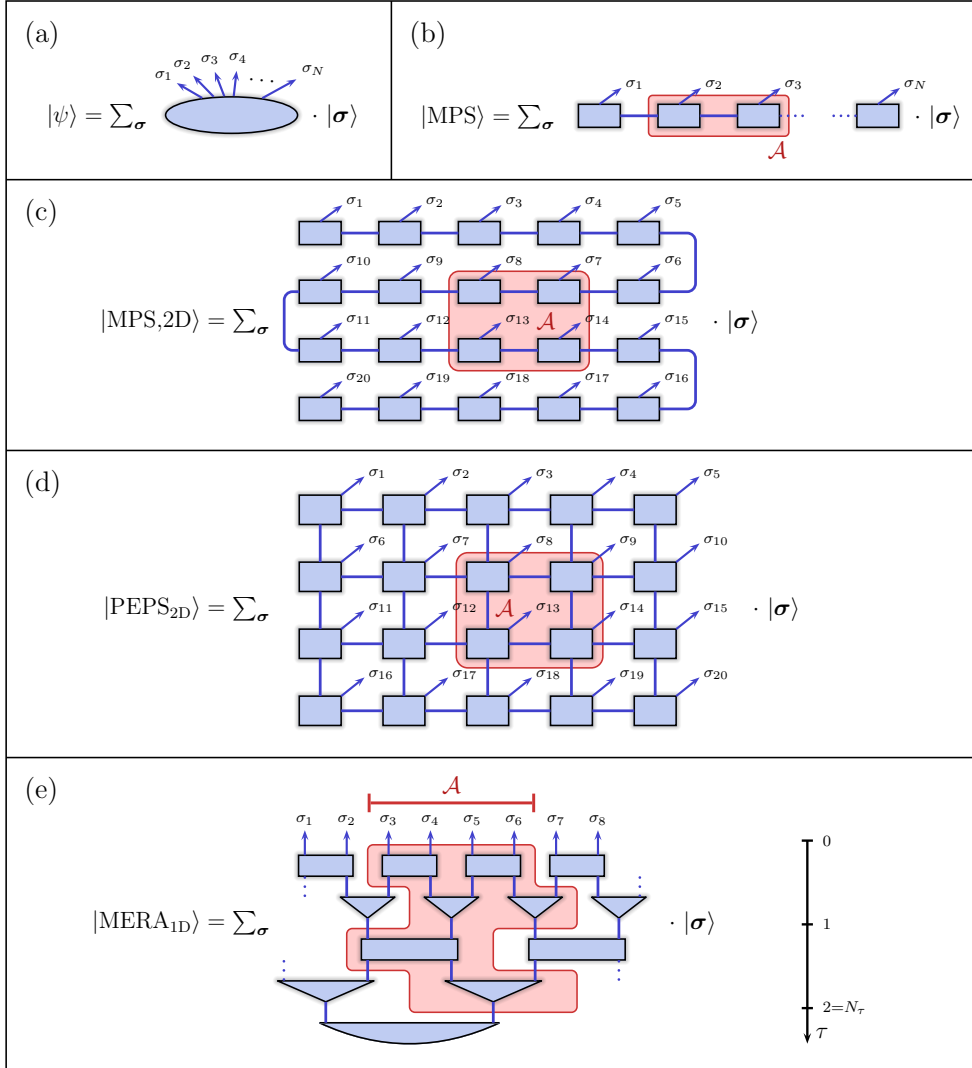


Figure 1.1.: (a) General state encoded by d^N coefficients ψ_{σ} . (b-e) Different options for organizing the degrees of freedom in a tensor contraction state. (b) MPS encoded by N rank-3 tensors A_i with dimensions (χ_i, χ_{i+1}, d) . (c) Trying to use an MPS for describing 2D ground states fails. For a fixed refinement parameter χ , the maximum entanglement entropy $S_{\text{MPS}}^{\text{max}}$ for subsystem $\mathcal{A}$ does not increase when $\mathcal{A}$ is stretched in the horizontal direction, although the entanglement in ground states actually scales with the surface area of $\mathcal{A}$ (up to logarithmic corrections). (d) 2D PEPS encoded by N rank-5 tensors with dimensions $(\chi, \chi, \chi, \chi, d)$ for the bulk of the system, and tensors of correspondingly lower rank for the open boundaries of the system. (e) 1D MERA encoded by rank-4 tensors that represent disentangling unitaries and rank-3 tensors that represent projecting isometries. The different layers τ of the MERA can be interpreted as realspace renormalization steps. In each step, the number of sites is halved.

1.4. Entanglement entropy in physical states of interest

Entanglement entropy quantifies quantum nonlocality for pure states; see Sec. 1.1. For a system divided into two subsystems $\mathcal{A}$ and $\mathcal{B} = \mathcal{L} \setminus \mathcal{A}$, containing $N_{\mathcal{A}}$ and $N_{\mathcal{B}}$ sites, respectively, the entanglement entropy for the state $|\psi\rangle$ is defined as the von Neumann entropy of the subsystem density matrix, i.e.,

$$S_{\mathcal{A}}(\psi) = -\text{Tr} \hat{\rho}_{\mathcal{A}} \log_2 \hat{\rho}_{\mathcal{A}} \quad \text{where} \quad \hat{\rho}_{\mathcal{A}} = \text{Tr}_{\mathcal{B}} |\psi\rangle\langle\psi|, \quad (1.5)$$

and $S_{\mathcal{A}} = S_{\mathcal{B}}$. The entropy equals zero for product states; $S_{\mathcal{A}}(|\psi_{\mathcal{A}}\rangle \otimes |\psi_{\mathcal{B}}\rangle) = 0$. States that maximize the entropy are of the form $|\phi\rangle = \sum_{i=1}^{N_{\min}} |i_{\mathcal{A}}\rangle \otimes |i_{\mathcal{B}}\rangle / \sqrt{N_{\min}}$ with $N_{\min} = \min(N_{\mathcal{A}}, N_{\mathcal{B}})$ and sets $\{|i_{\mathcal{A},\mathcal{B}}\rangle\}$ of orthonormal states on the subsystem Hilbert spaces $\mathcal{H}_{\mathcal{A}}$ and $\mathcal{H}_{\mathcal{B}}$, respectively. They are called *maximally entangled* and yield the maximum entanglement entropy $S_{\mathcal{A}}(\phi) = \log_2 d^{N_{\min}} = \log_2 d \cdot N_{\min}$. For our purposes, it is most interesting to look at simply connected subsystems. For this case, the maximum entanglement entropy for a subsystem $\mathcal{A}$ of linear size ℓ in a D -dimensional lattice (e.g., a hypercube of edge length ℓ , or ball of radius ℓ) in a larger environment $\mathcal{B}$ is

$$S^{\max}(\ell, D) = \log_2 d \cdot N_{\mathcal{A}} = \mathcal{O}(\ell^D), \quad (1.6)$$

i.e., proportional to the subsystem volume. States with an extensive entanglement entropy dominate in the Hilbert space. When one draws pure states $|\psi\rangle \in \mathcal{H}_{\mathcal{A}} \otimes \mathcal{H}_{\mathcal{B}}$ randomly according to the Haar measure, those states are with high probability close to a maximally entangled state [94].

In the following, the thermodynamic limit $N_{\mathcal{B}} \rightarrow \infty$ of a finite system $\mathcal{A}$ in an infinite environment $\mathcal{B}$ is assumed. It was mentioned before that systems of interest often do actually not exploit the (insurmountable) maximum number of degrees of freedom. This is reflected in the way the entanglement entropy scales with the subsystem size for the states of interest. A central result is that in ground states of gapped systems with short-range interactions, the entanglement entropy does not scale with the volume of the subsystem as in Eq. (1.6), but rather with the subsystem surface area as ℓ^{D-1} , which is called the *area law*, or as $\ell^{D-1} \log \ell$ for some cases of critical systems; see footnote 7 on critical points.

Ground states in 1D

For *non-critical* systems, the correlation length ξ is finite and the entanglement for a subsystem $\mathcal{A}$ of length ℓ with the rest of the system saturates for $\ell \gtrsim \xi$. This picture was confirmed in several numerical calculations. Exact results were for instance obtained for the XY model and the XXZ model in a transverse magnetic field, by Jordan-Wigner transformation, the Bethe Ansatz, or the corner transfer matrix method; see for example [95–97].

$$S_{\text{ID}}^{\text{gap}}(\ell) \xrightarrow{\ell \gtrsim \xi} S^*. \quad (1.7)$$

Only the surroundings (length scale ξ) of the edges of the subsystems contribute to their entanglement. Recently, this area law was proven on general grounds for gapped one-

dimensional models with finite-range interactions and a non-degenerate ground state [98] on the basis of Lieb-Robinson bounds [59–61].

For $\xi \gg 1$, i.e., *close to* a critical point, the long-range properties of the non-critical system can often be described by a massive $1 + 1$ -dimensional relativistic quantum field theory. Calculations in this framework [97] yield $S^* \sim \frac{c}{3} \log_2 \xi$. Here, c is the “conformal anomaly number” or “central charge” of the conformal symmetry that governs the system *at* the critical point.

At criticality (see footnote 7), the correlation length ξ diverges. As the energy gap vanishes, the corresponding field theory becomes “massless” and thus invariant under conformal transformations. The corresponding conformal field theories [99] are classified by the representations of the conformal group in $1 + 1$ dimensions, namely the central charges c and $\bar{c}$ of the holomorphic and the anti-holomorphic sectors.¹¹ As derived in Refs. [100, 101, 97], the entanglement entropy scales logarithmically with the linear subsystem size ℓ ,

$$S_{\text{ID}}^{\text{crit}}(\ell) = \frac{c}{3} \log_2 \ell. \quad (1.8)$$

Explicit calculations for the XY model and the XXZ chain [96] confirm this result.

Ground states in D dimensions

For the case of *quasi-free fermionic* models, it was shown in Ref. [102] that for both the critical and the non-critical case,

$$S_{\text{Fermi}}(\ell, D) \sim \ell^{D-1} S(\ell, 1), \quad (1.9)$$

holds when the subsystem $\mathcal{A}$ is a D -dimensional cube. For the critical case, one can indeed give lower and upper bounds to the entropy, proving that the area law is violated by a logarithmic factor [103, 102]

$$\mathcal{O}(\ell^{D-1} \log_2 \ell) \leq S_{\text{Fermi}}^{\text{crit}}(\ell, D) \leq \mathcal{O}(\ell^{D-1} (\log_2 \ell)^2). \quad (1.10)$$

Assuming (without proof) that the Widom conjecture [104] can be applied to the given case, Gioev and Klich derived further the dependence of the prefactor on the system parameters [102], finding

$$S_{\text{Fermi}}^{\text{crit}}(\ell, D) = \frac{\ell^{D-1} \log_2 \ell}{(2\pi)^{D-1}} \cdot \frac{1}{12} \int_{\partial\Omega} dS_x \int_{\partial\Gamma} dS_k |\mathbf{n}_x \cdot \mathbf{n}_k| + o(\ell \log_2 \ell), \quad (1.11)$$

where Ω is the real-space region of $\mathcal{A}$, rescaled by ℓ such that $\text{Vol}(\Omega) = 1$. Vectors $\mathbf{n}_x$ and $\mathbf{n}_k$ denote the normal vectors on the real-space surface $\partial\Omega$ and the Fermi surface $\partial\Gamma$.

¹¹The classification concerns the representations of the Virasoro algebra which is the algebra of the generators of local conformal transformations. The conformal symmetries (including translations, rotations, and scalings) in $1+1$ dimensions are so restrictive that several computations are considerably simplified. For example, two-point correlators of “quasi-primary” fields are fixed by the symmetries up to a scalar coefficient.

This is confirmed numerically with high accuracy in Chapter 3 and in the corresponding Refs. [105, 106].

For *quasi-free bosonic models* and specific subsystem geometries, early field theoretical and numerical calculations [107–109] indicated that the area law is obeyed both for the gapped as well as the critical case. This is confirmed by the derivation of bounds on the entropy [110, 111] for gapped systems, and by numerical calculations in the critical case in Chapter 3 and Ref. [105].

Time-evolved states

Calabrese and Cardy [112] examined the evolution of entanglement entropy for a pure state which is *not* an eigenstate of the (critical) Hamiltonian in the framework of 1+1-dimensional conformal field theory. They found linear increase of entanglement with time for $t < \ell/2$ and saturation to a value $\propto \ell$ for $t > \ell/2$.

$$S_{\text{ID}}^{\text{crit}}(\ell, t) \propto \begin{cases} t & \text{for } t < \ell/2 \\ \ell & \text{for } t > \ell/2 \end{cases} \quad (1.12)$$

Here, logarithmic corrections in the subsystem length ℓ have been omitted and units chosen such that the maximum propagation speed of excitations is equal to one. To make sure that this is not solely a feature of critical systems, the authors also inspect the spin- $\frac{1}{2}$ Ising chain in a transverse magnetic field at and away from the critical field $h = 1$. Another quite general result was presented in Ref. [113], where an upper bound on the evolving entanglement entropy is given which is linear in time. Chapter 5 and Ref. [114] designate conditions for both fermionic and bosonic quasi-free D -dimensional systems for which the entanglement entropy converges to an *extensive* value due to a dephasing effect, i.e.,

$$\lim_{t \rightarrow \infty} S^{\text{dephase}}(\ell, t, D) = \dots \propto \ell^D \quad (1.13)$$

which is the worst possible scaling as in Eq. (1.6).

For further details on entanglement entropy in many-particle systems, the interested reader is referred to the recent review [115]. In the following section, the presented results allow us to estimate how the number of degrees of freedom in a particular tensor contraction state needs to be scaled with system size or time, in order to obtain the correct scaling of entanglement entropy, necessary to accurately describe the simulated system.

1.5. Promising classes of tensor contraction states and their entanglement properties

In Sec. 1.3, the potential use of tensor contraction states for the simulation of many-particle quantum systems, particularly two-dimensional models, was motivated. Compared to an exact description, the degrees of freedom in those ansatz states are reduced in such a way that many physical states of interest can still be described with a high accuracy at

manageable computational costs. Here, several important examples for such classes of states are presented and it is discussed how the substantially reduced number of degrees of freedom has to be scaled with the system size in order to realize the scaling of entanglement entropy as occurring in non-critical or critical ground states, or during time evolution.

First, the tensor contraction states which are of interest to this thesis are introduced and upper bounds on the entanglement entropy, that can be encoded with those states, are derived.

Matrix product states

For MPS [83–85], which are also known as finitely-correlated states and which are illustrated in Fig. 1.1b, the expansion coefficients $\psi_{\sigma} = \langle \sigma | \psi \rangle$ of the many-particle state with respect to a basis of product states $|\sigma\rangle = |\sigma_1 \dots \sigma_N\rangle$ are chosen as a product of matrices $A_i^{\sigma_i}$ with sizes $\chi_i \times \chi_{i+1}$. For each lattice site, there are d of such matrices; see Eq. (1.4). In other words, whereas the expansion coefficients for an arbitrary state are encoded as a single tensor of rank N where all indices have dimension d , in an MPS, the expansion coefficients are given by N tensors A_i of rank three with dimensions (χ_i, χ_{i+1}, d) . The indices one and two of the tensor for a site i are contracted with indices two and one of the tensors A_{i-1} and A_{i+1} . Note that, in order to define the MPS for a given lattice it is necessary to define an ordering of the lattice sites. The dimensions χ_i , the *refinement parameters*, are typically chosen constant in the bulk of the system. The number of degrees of freedom $\sim d\chi^2 N$ is for fixed χ linear in the system size instead of exponential.

An upper bound for the maximum possible entanglement entropy $S_{\text{MPS}}^{\max}(i, j)$ for a splitting of the full system into a block $\mathcal{A}$ of sites $\{i, i+1, \dots, j\}$, contiguous in the chosen ordering, and the rest $\mathcal{B}$, is given by

$$S_{\text{MPS}}^{\max}(i, j) = \log_2 \chi_i + \log_2 \chi_j. \quad (1.14)$$

This is seen as follows: The MPS (1.4) can be written as

$$|\psi\rangle = \sum_{\alpha=1}^{\chi_i} \sum_{\beta=1}^{\chi_j} \sum_{\sigma} ([A_i^{\sigma_i} \dots A_j^{\sigma_j}]_{\alpha, \beta} \cdot |\sigma_i \dots \sigma_j\rangle) \otimes ([A_{j+1}^{\sigma_{j+1}} \dots A_{i-1}^{\sigma_{i-1}}]_{\beta, \alpha} \cdot |\sigma_{j+1} \dots \sigma_{i-1}\rangle) \quad (1.15)$$

$$=: \sum_{\alpha=1}^{\chi_i} \sum_{\beta=1}^{\chi_j} |\alpha\beta_{\mathcal{A}}\rangle \otimes |\alpha\beta_{\mathcal{B}}\rangle \stackrel{\text{SVD}}{=} \sum_{m=1}^{\chi_i \chi_j} \lambda_m |m_{\mathcal{A}}\rangle \otimes |m_{\mathcal{B}}\rangle. \quad (1.16)$$

The states $\{|\alpha\beta_{\mathcal{A}}\rangle\}$ and $\{|\alpha\beta_{\mathcal{B}}\rangle\}$ are defined by the matrix elements inside the parentheses of the first two lines. They are neither orthogonal nor normalized, and span $\chi_i \chi_j$ -dimensional subspaces of $\mathcal{H}_{\mathcal{A}}$ and $\mathcal{H}_{\mathcal{B}}$, respectively. Introducing orthonormal bases $\{|a_{\mathcal{A}}\rangle\}$ and $\{|b_{\mathcal{B}}\rangle\}$ for those subspaces, the last equality results from a singular value decomposition (SVD) of the $\chi_i \chi_j \times \chi_i \chi_j$ matrix Ψ with

$$\Psi_{ab} = \sum_{\alpha=1}^{\chi_i} \sum_{\beta=1}^{\chi_j} \langle a_{\mathcal{A}} | \alpha\beta_{\mathcal{A}} \rangle \langle b_{\mathcal{B}} | \alpha\beta_{\mathcal{B}} \rangle \stackrel{\text{SVD}}{=} \sum_{m=1}^{\chi_i \chi_j} \langle a_{\mathcal{A}} | m_{\mathcal{A}} \rangle \lambda_m \langle b_{\mathcal{B}} | m_{\mathcal{B}} \rangle. \quad (1.17)$$

Hence, the states $\{|m_{\mathcal{A}}\rangle\}$ and $\{|m_{\mathcal{B}}\rangle\}$ are orthonormal and the $\chi_i \chi_j$ nonzero eigenvalues of the subsystem density matrix are given by λ_m^2 . The maximum entanglement entropy for the given bipartition of the system, that can be encoded by the MPS, is given for the case where all λ_m^2 have the value $1/\chi_i \chi_j$. Using the definition (1.5), this yields $S_{\text{MPS}}^{\max}(i, j) = \sum_{m=1}^{\chi_i \chi_j} (\chi_i \chi_j)^{-1} \log_2(\chi_i \chi_j)$, i.e., Eq. (1.14).

Projected entangled-pair states

As we will see below, MPS are well suited for the simulation of 1D systems but generally fail for higher dimensions. Their suitable generalization to $D > 1$ is given by *tensor product ansätze* [116–118], also known as *projected entangled pair states* (PEPS) [119] and illustrated in Fig. 1.1d. As for MPS in 1D, the PEPS is encoded by assigning a tensor of rank $z+1$ and size $d\chi^z$ to each lattice site. Here, z denotes the lattice coordination number, the number of nearest neighbors for each site. Each tensor is contracted with the tensors of all neighboring sites (indices of dimension χ) and has one open index (dimension d), corresponding to the physical Hilbert space of that site. In a way, the tensor contractions encode the correlations in the system – similar to the multiplications of transfer matrices.

An upper bound for the maximum possible entanglement entropy $S_{\text{PEPS}}^{\max}(\mathcal{A})$ for a splitting of the full system into a subsystem $\mathcal{A}$, and the rest $\mathcal{B}$, is given by

$$S_{\text{PEPS}}^{\max}(\mathcal{A}) = |\partial\mathcal{A}| \log_2 \chi, \quad (1.18)$$

where $|\partial\mathcal{A}|$ denotes the surface area of the subsystem $\mathcal{A}$, or more precisely, the number of tensor contractions cut by the bipartition, see Fig. 1.1d. For a continuous block of linear size ℓ , it is $\propto \ell^{D-1}$, corresponding to the area law discussed in Sec. 1.4. The result (1.18) can be obtained in the same way as for the MPS by a Schmidt decomposition

$$|\psi\rangle = \sum_{\gamma=1}^{\chi^{|\partial\mathcal{A}|}} \sum_{\sigma, \sigma'} A_{\gamma}^{\sigma} B_{\gamma}^{\sigma'} |\sigma_{\mathcal{A}}\rangle \otimes |\sigma'_{\mathcal{B}}\rangle \stackrel{\text{SVD}}{=} \sum_{m=1}^{\chi^{|\partial\mathcal{A}|}} \lambda_m |m_{\mathcal{A}}\rangle \otimes |m_{\mathcal{B}}\rangle. \quad (1.19)$$

Multiscale entanglement renormalization ansatz

Another class of ansatz states is given by the *multiscale entanglement renormalization ansatz* (MERA) [120]. A MERA is also given by a set of partially contracted tensors. The particular form is motivated by a real-space renormalization picture. For each renormalization step, nearest-neighbor unitaries act on the lattice, followed by isometries which reduce the number of sites (corresponding to Kadanoff's spin block transformation [34]), yielding a new lattice with less sites. The unitaries are supposed to optimally disentangle those sites from the rest of the system that are projected onto a single site of the new lattice by the following isometry. For a finite D -dimensional lattice system with L^D sites and $L = z^{N_{\tau}}$, where in each renormalization step, the number of sites reduces by a factor z^D , the renormalization procedure ends after N_{τ} steps, i.e., the corresponding MERA

1. Introduction and overview

consists of N_τ layers of tensors, see Fig. 1.1e. In such a construction, the number of tensor contractions cut by the boundary $\partial\mathcal{A}$ of a bipartition is roughly given by

$$\frac{S_{\text{MERA}}^{\max}(\mathcal{A})}{\log_2 \chi} \sim \sum_{\tau=0}^{N_\tau-1} q^\tau |\partial\mathcal{A}| = \begin{cases} N_\tau |\partial\mathcal{A}| = |\partial\mathcal{A}| \log_z L & \text{for } D = 1 \\ |\partial\mathcal{A}|^{\frac{1-q^{N_\tau}}{1-q}} \rightarrow \frac{|\partial\mathcal{A}|}{1-q} & \text{for } D > 1 \end{cases} \quad (1.20)$$

where $q = 1/z^{D-1}$. So also for MERA, in $D > 1$, the upper bound on the entanglement entropy is proportional to the surface area $|\partial\mathcal{A}|$ of the subsystem. In $D = 1$, it contains the factor $\log_z L$, where L is the linear size of the *full* system $\mathcal{A} \cup \mathcal{B}$.

Scaling of entanglement entropy versus scaling of the refinement parameter χ

The (maximum) scaling of the entanglement entropy $S^{\max}(\chi)$ in the ansatz states, derived above, is to be compared to the scaling of the entanglement S in the physical states of interests, discussed in Sec. 1.4. There, S was often given as a function of the linear subsystem size ℓ . Choosing in the comparison for finite systems of total linear size L a linear subsystem size $\ell = \mathcal{O}(L)$, one obtains the relation between χ and L . This yields the following very rough scaling relations. The scaling of χ determines to a large extent the computational costs for ground state and time-evolution algorithms as those are polynomial in χ .

Situation	Entanglement	χ_{PEPS}	χ_{MERA}
$D \geq 1$, random state	$S(\ell) \sim \ell^D \log_2 d$	$\propto d^L$	$\propto d^{(1-q)L}$
$D = 1$, non-critical	$S(\ell) \rightarrow S^* \sim \frac{c}{3} \log_2 \xi$	$\propto \xi^{c/6}$	$\propto \xi^{c/(6N_\tau)}$
$D = 1$, critical	$S(\ell) \sim \frac{c}{3} \log_2 \ell$	$\propto L^{c/6}$	$\propto 2^{c/6}$
$D > 1$, free fermions, non-critical	$S(\ell) \sim \gamma \ell^{D-1}$	$\propto 2^\gamma$	$\propto 2^{(1-q)\gamma}$
$D > 1$, free fermions, critical	$S(\ell) \sim \gamma \ell^{D-1} \log_2 \ell$	$\propto L^\gamma$	$\propto L^{(1-q)\gamma}$
$D > 1$, free bosons	$S(\ell) \sim \gamma \ell^{D-1}$	$\propto 2^\gamma$	$\propto 2^{(1-q)\gamma}$
$D \geq 1$, time evolution	$S(\ell, t) \sim \gamma t \ell^{D-1}$	$\propto 2^{\gamma t}$	$\propto 2^{(1-q)\gamma t}$
$D \geq 1$, steady state	$S(\ell, \infty) \sim \gamma \ell^D$	$\propto 2^{\gamma L}$	$\propto 2^{(1-q)\gamma L}$

The variable q , occurring in the column for the MERA refinement parameter χ_{MERA} , is defined as above as $q = 1/z^{D-1}$, where z^D is the factor by which the number of sites reduces in each renormalization step. The column “ χ_{PEPS} ” states, for spatial dimensions $D > 1$, the scaling of the refinement parameter χ for a PEPS and, for $D = 1$, its scaling for an MPS, which is basically a 1D version of the PEPS. The table states rough scaling relations for the required χ . For more precise relations one needs to consider the full spectra of the subsystem density matrices as in Refs. [95, 121], not merely their entropy.

The DMRG and hence MPS have also been applied for 2D systems [122, 123]. For this purpose, one chooses a certain ordering of the sites and puts the MPS onto the lattice accordingly, see Fig. 1.1c. This approach is however not efficient when the entanglement entropy obeys an area law: In the example of Fig. 1.1c the subsystem $\mathcal{A}$ is rectangular. Let the edge lengths be labeled ℓ_x and ℓ_y . With an area law, the subsystem entropy is

proportional to the surface $2(\ell_x + \ell_y)$. For the MPS, an upper bound for the entanglement entropy is however given by $2\ell_y \log \chi$. As in Eq. (1.14), it is proportional to the number of tensor contractions cut by the bipartition. Hence the refinement parameter χ needs to be scaled exponentially in the horizontal extension L_x of the system.

According to the comparison in the table above, algorithms on MPS (for 1D), PEPS, and MERA are generally efficient for the simulation of non-critical ground states. For critical 1D systems, χ_{PEPS} needs to be scaled with a (small) power of the system size L . In this case, the MERA states are favorable since χ can be kept constant when increasing the system size. For $D > 1$, this advantage of the MERA is most likely lost, as both MERA and PEPS obey an area law in this case.

However, the situation is less fortunate for time-evolved states, e.g., after quenches of system parameters as considered in Chapter 5. The typically linear increase of S in time and, for the steady state, the extensive scaling of S with the subsystem size ℓ require an exponential scaling of the refinement parameter χ with t and L . Therefore, in time-evolution simulations there is usually a maximum time at which the simulation needs to be stopped, because entanglement entropy has grown to an extent that makes it infeasible to continue representing the state of the system, with a given small deviation tolerance, in form of an MPS, PEPS, or MERA with the given limited computer resources. See however Chapter 6 for an application where this problem can be circumvented almost completely.

Optimization algorithms

To obtain a ground state, the tensor contraction states, introduced above, are typically optimized by iterative variation of the energy functional where, as in DMRG, a small set of tensors is optimized in each step, or some form of imaginary time evolution is implemented, see, e.g., [66, 124, 74, 81, 119, 125–129]. For all algorithms, the computational costs scale polynomially in the refinement parameter χ .

The considerations about how χ is to be scaled with the system size naturally only apply to simulations of finite-size systems. However, several algorithms work directly in the thermodynamic limit [80, 81, 126, 127, 129]. For such simulations at a critical point (except for the case of the 1D MERA), the finite refinement parameter χ induces an effective finite correlation length $\xi \sim \chi^\kappa$ [130, 131] just like other perturbations.

There are further classes of tensor contraction states which, due to a lack of locality in the organization of the degrees of freedom, do not allow for an optimization in the above sense, see, e.g., [132–134]. Such states are then typically optimized by Monte Carlo techniques as in the traditional VMC method mentioned in Sec. 1.2. Algorithms for PEPS and MERA scale polynomially in χ , but the leading power is already relatively high for the 2D case. Hence, Monte Carlo optimization of those states is also a useful option.

1.6. Content of the thesis and outlook

The first part of this work, extends the current knowledge on the scaling of entanglement entropy in many-particle ground states, especially at criticality. The scaling of entanglement is derived within the framework of 1+1-dimensional boundary conformal field theory, see Chapter 2. Instead of the von Neumann entropy, Rényi entropies are used, generalizing the result (1.8). A special focus lies on the effect of the boundary conditions which result in different additive constants to the entropy. Majorization relations for the spectra of the subsystem density matrix are shown to hold along renormalization group flows. Exact numerics for the scaling of entanglement entropy in critical 2D Fermi and Bose systems are presented in Chapter 3. The scaling behavior, Eq. (1.11), for critical fermionic systems, as conjectured in the literature, is confirmed to a high precision. For the special case, where the Fermi surface of the critical system is zero-dimensional, an area law with a sublogarithmic correction is observed. Calculations for critical Bose systems confirm earlier indications for an area law. Whereas, in the rest of the thesis, translation invariant models in finite spatial dimensions are considered, the entanglement scaling in “collective” systems with an infinite lattice coordination number, or, equivalently, infinite dimension is discussed in Chapter 4 together with some applications. At the critical point, the entanglement is found to scale logarithmically with the subsystem size.

It is investigated in Chapter 5 how integrable models evolve in time, particularly in what sense and due to what effect they can converge to a steady state. Sufficient preconditions, examples, and counter-examples for such a convergence are given. The steady states differ from the typical canonical ensembles: Due to the large number of integrals of motion they carry memory of the initial states. The entanglement entropy in the steady states is found to be extensive, i.e. proportional to the subsystem size; see Eq. (1.13).

The second part of the thesis, focuses on the simulation techniques employing tensor contraction states. In Chapter 6, a new MPS (DMRG) method is presented that allows for the precise determination of finite temperature spectral functions. In order to simulate a finite temperature state, a purification is used. The limitation to finite physical times, which occurs due to the growth of the entanglement entropy, is circumvented by continuation of the measured observables via linear prediction to infinite times. The method is benchmarked versus exact Bethe ansatz calculations for $T = 0$ and QMC for finite temperatures. The proposed method seems to be favorable compared to the QMC approach, since it avoids an ill-conditioned analytical continuation of the spectral function from the imaginary to the real-time axis, as well as sign problems.

The PEPS and MERA simulation algorithms for higher-dimensional systems, as addressed in the previous section, are actually limited to the case of spin models. However, several models of high interest, such as the 2D Fermi Hubbard model, are fermionic. In principle, one could apply a Jordan-Wigner transformation in order to map the fermion model to a spin model. But such transformations generate unfavorable nonlocal Jordan-Wigner string operators which completely spoil the efficiency of the algorithms for PEPS and MERA. To solve this problem, a fermionic variant of the MERA is introduced in Chapter 7 and nonlocal operators are avoided by dynamically changing the particular mode

ordering, chosen for the Jordan-Wigner representation, after each renormalization stage in the fermionic MERA. In Chapter 8, this solution is developed into a general method that allows to simulate the fermionic version of any spin tensor contraction state with the *same* computational cost as for the corresponding spin case, up to marginal overheads. The major part of the chapter applies to tensor contraction states in general. As a specific example it is described in some detail how a spin PEPS algorithm needs to be modified for simulations of fermionic systems.

Needless to say, there is much room for future research. Much of our knowledge about the scaling of quantum nonlocality is based on quasi-free models. It is an important task to add further results for interacting systems. The novel numerical approaches based on tensor contraction states, especially those for fermions as developed in this thesis, provide new routes to some long-standing questions on quantum many-particle systems of technological relevance – e.g., the phenomena of high-temperature superconductivity, or frustrated magnetism. The scaling of the number of degrees of freedom and computational cost seem to be manageable. Further research in this matter is concerned with the optimization of the numerical algorithms for the specific needs of their applications in order to achieve good convergence and reasonable computation times.

Part I.

Scaling of entanglement entropy in many-particle systems

2. Entanglement and boundary critical phenomena

Boundary critical phenomena are investigated from a quantum information perspective. Bipartite entanglement in the ground state of one-dimensional quantum systems is quantified using the Rényi entropy S_α , which includes the von Neumann entropy ($\alpha \rightarrow 1$) and the single-copy entanglement ($\alpha \rightarrow \infty$) as special cases. The contribution from the boundary entropy to the Rényi entropy is identified, and entanglement loss along boundary renormalization group (RG) flows is derived. This property, which is intimately related to the Affleck-Ludwig g -theorem, can be regarded as a consequence of majorization relations between the spectra of the reduced density matrix along the boundary RG flows. It is also pointed out that the bulk contribution to the single-copy entanglement is half of that to the von Neumann entropy, whereas the boundary contribution is the same.

Recently much work has been done to understand entanglement in quantum many-body systems. In particular, the behavior of various entanglement measures at or near a quantum phase transition [57, 58] has received a lot of attention; see Sec. 1.4 and Refs. [135–137, 96, 97, 101, 138–144]. These entanglement measures include the von Neumann entropy and the single-copy entanglement, among others. The former is the most studied measure and quantifies entanglement in a bipartite system in the so-called asymptotic regime [145], whereas the latter was recently suggested to quantify the entanglement present in a single copy [144]. For a system in a pure state $|\psi\rangle$ (e.g., the ground state) that is partitioned into two subsystems $\mathcal{A}$ and $\mathcal{B}$, the von Neumann entropy is

$$S_1 \equiv -\text{Tr}_{\mathcal{A}} \rho_{\mathcal{A}} \log_2 \rho_{\mathcal{A}} \quad (2.1)$$

where $\rho_{\mathcal{A}} = \text{Tr}_{\mathcal{B}} |\psi\rangle\langle\psi|$ is the reduced density matrix for $\mathcal{A}$, and the single-copy entanglement is $S_\infty \equiv -\log_2 \lambda_1$, where λ_1 is the largest eigenvalue of $\rho_{\mathcal{A}}$.

Studies of the von Neumann entropy for quantum spin chains [137, 96, 97, 101, 138–142] have revealed that its dependence on the size ℓ of the block $\mathcal{A}$ is very different for noncritical and critical systems. For the former, the von Neumann entropy increases logarithmically with ℓ until it saturates when ℓ becomes of order the correlation length ξ , while for the latter (having $\xi = \infty$) it diverges logarithmically with ℓ . Remarkably, the prefactor of the logarithmic term is universal and proportional to the central charge of the underlying conformal field theory (CFT) [100, 97]. Furthermore, it has been shown numerically [146] that the *entanglement loss* along the (bulk) renormalization group (RG) flows, which is consistent with the CFT predictions for the von Neumann entropy [97, 100] and with Zamolodchikov’s c -theorem [147], can be given a more “fine-grained” characterization in

terms of the *majorization* concept [148]. A theoretical analysis of majorization in these systems also appeared recently [149].

Boundary critical phenomena [150] in one-dimensional (1D) quantum systems (equivalently, 2D classical systems) have attracted a lot of interest, especially in the context of boundary CFT. A closely related subject is the theory of boundary perturbations of certain conformally invariant theories, so-called integrable boundary quantum field theory [151], which is relevant to quantum spin chains with nontrivial boundary interactions, impurities in Luttinger liquids, Kondo physics, tunneling in fractional quantum Hall devices, and open string theory. In these problems, the Affleck-Ludwig g -theorem [152, 153] plays a similar role as the c -theorem does for bulk critical phenomena.

This chapter presents an investigation of boundary critical phenomena in quantum spin chains from a quantum information perspective. The findings provide new insights into the information-theoretic explanation of the boundary entropy and the g -theorem characterizing the intrinsic irreversibility due to information loss along boundary RG flows [154]. The Rényi entropy (also known as the α -entropy),

$$S_\alpha = (1 - \alpha)^{-1} \log_2 \text{Tr}_A \rho_A^\alpha, \quad (2.2)$$

is used as an entanglement measure, partly motivated by the fact that both the von Neumann entropy and the single-copy entanglement are special cases of the Rényi entropy, corresponding to $\alpha \rightarrow 1$ and $\alpha \rightarrow \infty$, respectively. Using CFT expressions for the Rényi entropy are derived which include a boundary entropy contribution, and it is shown that a majorization relation underlies an entanglement loss along boundary RG flows (i.e., when a system with a boundary interaction flows from an unstable to a stable fixed point). The analytical arguments are supported with numerical density-matrix renormalization group (DMRG) calculations [66, 68].

2.1. Rényi entropy and conformal field theory

Consider a 1D lattice of interacting spins with lattice spacing a . Let L be the total length of the system, and let the two subsystems $\mathcal{A}$ and $\mathcal{B}$ be blocks of consecutive spins of length ℓ and $L - \ell$, respectively. Then CFT predicts that for an infinite spin chain at criticality,

$$S_\alpha = \frac{c}{6} (1 + \alpha^{-1}) \log_2 \frac{\ell}{a} + c'_\alpha \quad (2.3)$$

where c is the central charge and c'_α is a non-universal constant [97]. For a semi-infinite spin chain with the block $\mathcal{A}$ starting at the origin where a boundary interaction is applied, we have instead

$$S_\alpha = \frac{c}{12} (1 + \alpha^{-1}) \log_2 \frac{2\ell}{a} + \frac{1}{2} c'_\alpha + S_b. \quad (2.4)$$

Here $S_b = \log_2 g$ is the boundary entropy [152, 153], with $g = \langle B|0\rangle$, where $|B\rangle$ is a boundary state [155, 156, 99]¹ and $|0\rangle$ is the ground state. It is emphasized that, compared

¹The boundary states are also well-defined for systems off criticality, see Ref. [151].

with the corresponding expression for S_1 in Ref. [97], there is an extra factor $1/2$ in front of c'_α and S_b in Eq. (2.4).

The corresponding Rényi entropies for finite L are found from Eqs. (2.3) and (2.4) by standard conformal mappings [99]. As a result, the Rényi entropy for periodic boundary conditions (PBC) [open boundary conditions (OBC)] is given by replacing

$$\frac{\ell}{a} \mapsto \frac{L}{\pi a} \sin \frac{\pi \ell}{L} \quad (2.5)$$

in Eq. (2.3) [Eq. (2.4)]. For the OBC case it has been assumed that the BC on the left and right ends are identical; otherwise one has to consider the complicating effects of a boundary condition changing operator.

From these results one sees that the contribution of the *bulk* universal part to the single-copy entanglement S_∞ is always *half* of that to the von Neumann entropy S_1 , thus extending the conclusion in Ref. [144] for the XX chain ($c = 1$) to all conformally invariant critical systems. However, it is stressed that the contribution of the boundary entropy to S_α does not depend on α .

The details of the CFT derivation of the above results (which makes use of CFT expressions for $\text{Tr}_A \rho_A^\alpha$ from Ref. [97]) will be given elsewhere. Here, instead, a heuristic argument to justify Eqs. (2.3) and (2.4) is presented. As is well known, the central charge c , which measures the (effective) number of gapless excitations, describes the way a specific system reacts to the introduction of a macroscopic length scale into the system [99]. Therefore, when the entire (infinite) system is partitioned into a block of length ℓ and its environment, one may expect that the Rényi entropy S_α depends only on c and ℓ/a with some short distance cutoff a , e.g., the lattice spacing for quantum spin chains. Because both the Rényi entropy and the central charge are *additive*, one can see² that the Rényi entropy must be linear as a function of the central charge, *i.e.*, $S_\alpha = c f_\alpha(\ell/a) + h_\alpha$, with f_α a universal function and h_α a non-universal (*i.e.*, model-dependent) function. The specific form of the function f_α may be determined by calculating the Rényi entropy for any exactly solvable model, for instance the massless Dirac fermion field as done in Ref. [143] for PBC, thus confirming Eq. (2.3). The calculation may be extended to the massless Dirac fermion with a conformally invariant boundary, leading to the conclusion that h_α consists of the non-universal bulk part $1/2 c'_\alpha$ and the universal boundary part S_b . The bulk universal part of Eq. (2.4) and its counterpart for finite L result from the substitution $c \mapsto c/2$, $\ell \mapsto 2\ell$ and $L \mapsto 2L$ in Eq. (2.3) and its corresponding counterpart, due to the fact that one may “unfold” the system by identifying left-movers at position x ($x = ja$, with j labeling lattice sites) with right-movers at $-x$ so that the resulting system consists of only right movers subject to PBC and with the system size scales ℓ and L doubled and the number of gapless degrees of freedom halved. The factor $1/2$ in front of c'_α in the second bulk term in Eq. (2.4) also originates from this halving of the number of gapless degrees of freedom.

²For a composite system $\mathcal{AB}$ consisting of two non-interacting systems $\mathcal{A}$ and $\mathcal{B}$, one has $S_\alpha^{\mathcal{AB}}(c^{\mathcal{AB}}, \ell/a) = S_\alpha^{\mathcal{A}}(c^{\mathcal{A}}, \ell/a) + S_\alpha^{\mathcal{B}}(c^{\mathcal{B}}, \ell/a)$ and $c^{\mathcal{AB}} = c^{\mathcal{A}} + c^{\mathcal{B}}$. This implies that $S_\alpha^{\mathcal{A}}(c^{\mathcal{A}}, \ell/a) = c^{\mathcal{A}} f_\alpha(\ell/a) + h_\alpha^{\mathcal{A}}$. So f_α is not model-specific whereas h_α is.

2.2. $S = 1/2$ transverse Ising and XXZ chains in boundary magnetic fields

Let us now address the implications of these CFT predictions for models of semi-infinite quantum spin chains and let us first consider the $S = 1/2$ transverse Ising chain in a boundary magnetic field, described by

$$H_{\text{Ising}} = - \sum_{j=0}^{\infty} (S_j^x S_{j+1}^x + h S_j^z) + h_b S_0^x. \quad (2.6)$$

Here h is the transverse bulk magnetic field, and h_b is the boundary magnetic field. The field is set to $h = 1/2$ so that the model is bulk critical with central charge $c = 1/2$. The second model is the $S = 1/2$ XXZ chain, for which

$$H_{\text{XXZ}} = \sum_{j=0}^{\infty} (S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + \Delta S_j^z S_{j+1}^z) + h_b S_0^x. \quad (2.7)$$

Here Δ denotes the anisotropy and h_b is the (transverse) boundary magnetic field. The model is bulk critical with central charge $c = 1$ for $-1 < \Delta \leq 1$.

For both models, the points $h_b = 0$ and $h_b = \pm\infty$, corresponding to the free and fixed conformally invariant BC, are boundary critical fixed points; the former is unstable and the latter is stable. A boundary magnetic field $h_b > 0$ is generally a relevant perturbation of the free BC $h_b = 0$, and generates a boundary RG flow of h_b towards the fixed point $h_b = \infty$. For $0 < h_b < \infty$, the conformal invariance is lost, and the competition between boundary ordering and bulk criticality introduces a crossover length $\zeta \propto h_b^{d-1}$ [157], where $d < 1$ is the scaling dimension of the relevant boundary perturbation. For the Ising model, $d = 1/2$, and for the XXZ model, $d = 2\pi R^2$, where $R = \sqrt{(1/2\pi) - (1/2\pi^2) \arccos \Delta}$ is the compactification radius. Furthermore, for both models, g for fixed BC is less than g for free BC, which implies that the Rényi entropy is less for fixed than for free BC. This is also consistent with the g -theorem [152, 153], which states that g decreases along boundary RG flows. For the transverse Ising model, $g = 1$ (free) and $g = 1/\sqrt{2}$ (fixed) [155, 156]; for the XXZ model, $g = \pi^{-1/4}(2R)^{-1/2}$ (free) and $g = \pi^{1/4}R^{1/2}$ (fixed) [157]. It is emphasized that even away from boundary critical points, Eq. (2.4) is still valid for $\ell > \zeta$, due to bulk criticality.

H_{XXZ} reduces to the isotropic XXX (Heisenberg) model for $\Delta = 1$ ($R = 1/\sqrt{2\pi}$). This case is special, because the boundary perturbation is marginal ($d = 1$). In fact, $g = 2^{-1/4}$ for both free and fixed BC. The line from $h_b = 0$ to $h_b = \infty$ is a line of fixed points; there is no RG flow since g is the same everywhere along the line. To see this, let us consider the finite XXX chain with identical boundary interactions at the two boundaries. This corresponds to a free scalar boson field with a dynamical boundary interaction [158], for which it was found that when both ends have the same BC, the partition function is independent of the boundary interaction strength, reflecting the fact that the energy levels do not feel the presence of the boundary interaction. Combining this with the CFT prediction [159]

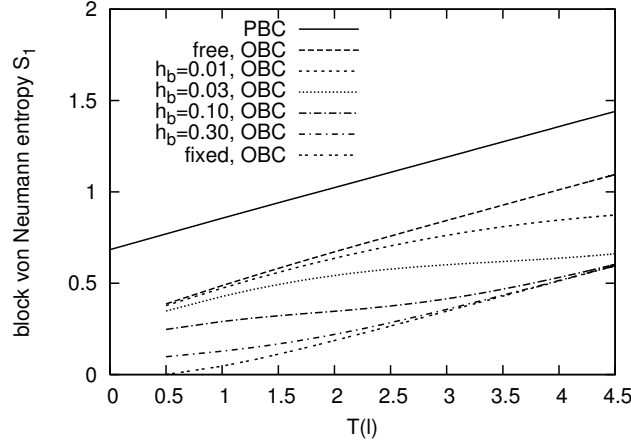


Figure 2.1.: Bipartite entanglement for the bulk critical transverse Ising model, quantified by the von Neumann entropy S_1 of the reduced density matrix. The block size ℓ is given as $T(\ell)$ (see text) which allows for a direct check of the CFT predictions (2.3) and (2.4). The fit yields the predicted boundary entropies.

$S = (\pi c/3\beta)L + 2S_b$ for the Gibbs entropy $S \equiv -\beta^2 \partial F / \partial \beta$, it is to be concluded that the boundary entropy does not depend on the boundary magnetic field h_b .

To check the CFT predictions, quasi-exact DMRG results are analyzed. Fig. 2.1 shows the entanglement in the bulk critical transverse Ising model (2.6) for PBC and OBC with different boundary fields h_b . For PBC the DMRG variant described in Ref. [160] is used. The block size ℓ is shown as $T(\ell)$, with

$$T_{\text{PBC}}(\ell) = \log_2 \left(\frac{L}{\pi a} \sin \frac{\pi \ell}{L} \right) \quad (2.8)$$

and

$$T_{\text{OBC}}(\ell) = \frac{1}{2} \log_2 \left(\frac{2L}{\pi a} \sin \frac{\pi \ell}{L} \right), \quad (2.9)$$

appropriate for a linear fit of the finite L counterparts of (2.3) and (2.4). The fits for PBC, free OBC and fixed OBC yield the desired central charge ($c = 0.500, 0.502, 0.498 \approx 1/2$) and the predicted boundary entropies ($S_b^{\text{free}} = -0.003 \approx 0$, $S_b^{\text{fixed}} = -0.497 \approx \log_2 1/\sqrt{2}$), which can be read off from the differences of the axis intercepts. The curves for nonzero h_b converge for large ℓ to the fixed BC curve (the smaller the value of h_b , the larger the crossover length ζ). This implies that the boundary entropy for any nonzero h_b is the same as that for fixed BC, consistent with the explicit construction of boundary states in Ref. [151].

2.3. Majorization relations

Let us first recall the definition of majorization [148]. Consider two probability distributions $\lambda \equiv \{\lambda_i\}$ and $\mu \equiv \{\mu_i\}$ whose elements are ordered such that $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_r$, and similarly for μ . The distribution λ is said to be majorized by μ , written $\lambda \prec \mu$, if $\sum_{i=1}^k \lambda_i \leq \sum_{i=1}^k \mu_i$ for $k = 1, \dots, r-1$ and $\sum_{i=1}^r \lambda_i = \sum_{i=1}^r \mu_i (= 1)$. Here the probability distributions are formed by the eigenvalues of the reduced density matrix $\rho_{\mathcal{A}}$, and r is the Schmidt rank. An elementary result [148] states that $\lambda \prec \mu$ if and only if $\phi(\lambda) \geq \phi(\mu)$ for all Schur-concave functions ϕ ³. In fact, the Rényi entropy is Schur-concave for any index α . Therefore it is necessary (but not sufficient) for the Rényi entropy for all indices α to be monotonic with some system parameter (ℓ or h_b) for the corresponding spectra of the reduced density matrix to be subject to a majorization relation.

The CFT results (2.3) and (2.4) show that at (both bulk and boundary) criticality the Rényi entropy increases monotonically with the block size ℓ (for this to hold for a finite chain of length L , ℓ must be less than $L/2$). In particular, the largest eigenvalue $\lambda_1 = 2^{-S_\infty}$ of $\rho_{\mathcal{A}}$ decreases with increasing ℓ . This indicates that $\rho_{\mathcal{A}'} \prec \rho_{\mathcal{A}}$ if the block $\mathcal{A}$ is a sub-block of $\mathcal{A}'$ ⁴. Indeed, the majorization relation follows from the fact that any two eigenvalue distributions, corresponding to two different block sizes, only cross *once* when the eigenvalues λ_i are plotted versus the eigenvalue index i . That is, an index i^* exists, such that λ_i decreases with increasing ℓ for $i \leq i^*$, and λ_i increases with increasing ℓ for $i > i^*$. The uniqueness of this crossing is guaranteed by the fact that the eigenvalue distribution follows $\lambda_i \propto q^{\beta_i}$ for both bulk and boundary conformal theories, apart from degeneracies n_i . Here $q = \exp(2\pi i\tau)$ for conformal theories and $q = \exp(-\pi\delta)$ for boundary conformal theories, and β_i are integers related to the scaling dimensions of the descendant operators. The conformal invariance requires that both τ and δ should be proportional to $1/\ln \ell$. The discreteness of n_i and β_i ensures that they do not change when the block size ℓ is varied (for finite L , ℓ must be restricted to even or odd values if the model has a parity effect).

Next, let us consider the behavior of the Rényi entropy along boundary RG flows. By combining the derived CFT results with the g -theorem, it follows that the Rényi entropy decreases (more precisely, does not increase) along boundary RG flows. In particular, the largest eigenvalue λ_1 of $\rho_{\mathcal{A}}$ increases along the boundary RG flow. Furthermore, one may argue that along the boundary RG flow, the eigenvalues of $\rho_{\mathcal{A}}$ take the same form $\lambda_i \propto q^{\beta_i}$ as at the conformally invariant fixed point at the end of the flow, except that the dependence of q on ℓ is different (again, the discreteness of the degeneracies n_i and β_i ensures that they remain the same along the flow). However, for any nonzero h_b , the bulk criticality requires that the dependence $\delta \sim 1/\ln \ell$ is recovered for $\ell > \zeta$. It then follows that there is *one and only one* crossing for the eigenvalue distributions versus i along the boundary RG flows.

³A function ϕ is Schur-concave if $\lambda \prec \mu \Rightarrow \phi(\lambda) \geq \phi(\mu)$.

⁴A rigorous proof for this fact was attempted in Ref. [149] for bulk conformal theories, where it was claimed that all eigenvalues except the largest one increases with increasing block size ℓ . This is not valid, as one can see from the exact solution for the XX model [95], which shows that the second largest eigenvalue first increases with ℓ before it starts decreasing. The turning point is at $\ell/a \sim 1800$.

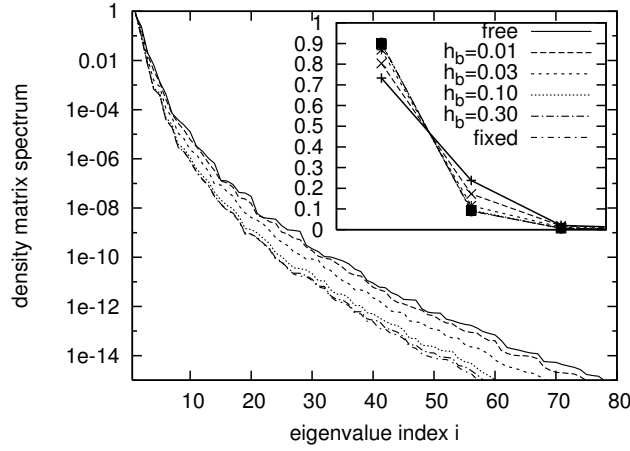


Figure 2.2.: Eigenvalue distributions for the reduced density matrix of a block of size $\ell = 128a$ in the bulk critical transverse Ising model (2.6) for various values of the boundary magnetic field h_b . The quasi-exact DMRG results confirm the majorization relation along the boundary field RG flow (see text). The inset shows that the crossing of the spectra occurs at $i^* = 1$.

More precisely, an index i^* exists, such that λ_i increases for $i \leq i^*$, and decreases for $i > i^*$ along the flows. This in turn implies the majorization relation.

A rough estimate for the crossing index i^* can be obtained from the CFT predictions for the largest eigenvalue λ_1 . This gives $i^* \sim \ell^{c/6}$ for PBC and $i^* \sim \ell^{c/12}$ for OBC. Thus the block size ℓ must be sufficiently large to observe that the crossing occurs at $i^* > 1$. For instance, to see that the second largest eigenvalue decreases with increasing ℓ , ℓ should at least be $1800a$ for the semi-infinite XX chain, as estimated from the exact solution [95]. DMRG calculations of the reduced density matrix spectra show majorization along boundary RG flows, where eigenvalues down to $\sim 10^{-15}$ are considered. Fig. 2.2 shows the crossing point i^* of the spectra in the bulk critical transverse Ising model with block size $\ell = 128a$ and various values of the boundary field h_b . The crossing of the spectra occurs here at $i^* = 1$.

For the Heisenberg XXX model ($\Delta = 1$) the Rényi entropy does not depend on the boundary magnetic field: $\partial S_\alpha / \partial h_b = 0$. These constraints (of which there is an infinite number, one for each α) imply that the spectra of ρ_A do not vary with h_b . Therefore the presence of a line of fixed points here amounts to the statement that all of these critical points share the same eigenvalue distribution, so there is no boundary RG flow (a boundary RG flow would require a preferential direction characterized by (strict) majorization).

2.4. Conclusions

In this chapter, the interrelations between the boundary entropy, the Affleck-Ludwig g -theorem and entanglement in quantum spin systems with boundary interactions have been investigated. The intrinsic irreversibility along boundary RG flows, as embodied in Affleck-Ludwig g -theorem, is connected with the majorization relation solely characterized by the ground state itself. The results will bring new insights into our understanding of 2D statistical mechanical systems with boundary interactions and (perturbed) conformal theories defined on manifolds with boundaries. The equivalence between 1D quantum systems and 2D classical systems indicates that majorization relations should still be preserved in 2D classical systems, even if it does not make sense to speak of quantum entanglement for classical cases.

During the preparation of this part of the thesis, two related works [161, 162] appeared which reached the same conclusion as here regarding the connection between the von Neumann entropy and the single-copy entanglement for bulk conformal theories.

3. Entanglement scaling in critical two-dimensional fermionic and bosonic systems

The reduced density matrices of quadratic fermionic and bosonic models are related to their Green's function matrices in a unified way and the scaling of the entanglement entropy of finite systems in an infinite universe is determined exactly. For critical fermionic 2D systems at $T = 0$, two regimes of scaling are identified: generically, one finds a logarithmic correction to the area law with a prefactor dependence on the chemical potential that confirms earlier predictions based on the Widom conjecture. If, however, the Fermi surface of the critical system is zero-dimensional, one finds an area law with a sublogarithmic correction. For a critical bosonic 2D array of coupled oscillators at $T = 0$, the numerical results show that the entanglement entropy follows the area law without corrections.

Entanglement is a key feature of the non-classical nature of quantum mechanics. It is a necessary resource for quantum computation and is at the heart of interesting connections between quantum information theory and traditional quantum many-body theory, such as in quantum critical phenomena [163, 137, 135] or the quantum Hall effect [164, 165].

One of the most widely used entanglement measures for pure states is the entropy of bipartite entanglement: For a pure state $|\Psi_{AB}\rangle$ of a bipartite "universe" AB consisting of system A and environment B it is given by the von Neumann entropy

$$S_A = -\text{Tr } \rho_A \log_2 \rho_A, \quad (3.1)$$

where $\rho_A = \text{Tr}_B |\Psi_{AB}\rangle\langle\Psi_{AB}|$ is the reduced density matrix of system A .

An important question is how the entanglement entropy scales at $T = 0$ with the size of the system, assuming the universe to be in the thermodynamic limit. This was first studied by Bekenstein in the context of black hole entropy [166]. As opposed to thermodynamic entropy, which is extensive, entanglement entropy was found to be proportional to the area of the black hole's event horizon, its physical locus being essentially the hypersurface separating system and environment. Entanglement entropy scaling hence depends decisively on the dimension d of the universe. As discussed in Sec. 1.4, this so-called area law has been extensively studied. In one dimension, $d = 1$, scaling is well understood both for fermions (or equivalently spins) [137, 138, 167] and bosons [168, 169]. For one-dimensional spin chains at $T = 0$, one finds that the entanglement entropy $S_A(L)$ of a system A of linear size L saturates away from criticality, but scales as $\log_2 L$ when the system becomes critical [137, 170, 140, 171, 141], i.e. when correlation lengths diverge.

In the latter case, conformal field theory (CFT) yields [101, 97]

$$S_{\mathcal{A}}(L) = \frac{c + \bar{c}}{6} \log_2 L + k, \quad (3.2)$$

where c and $\bar{c}$ are the holomorphic and the anti-holomorphic central charges of the field theory. Essentially, there is no physical limit to the boundary region between system and environment.

The situation is far less clear in higher dimensions $d > 1$. The area law implies that, away from criticality, the entanglement entropy is essentially proportional to the surface area of system $\mathcal{A}$

$$S_{\mathcal{A}} \sim L^{d-1}, \quad (3.3)$$

as confirmed in analytical calculations for (bosonic) non-critical coupled oscillators [110].

At criticality, the correlation lengths diverge and one may expect corrections to the area law, as for $d = 1$. For critical ground states of fermionic tight-binding Hamiltonians, the entanglement entropy was indeed found to scale as

$$S_{\mathcal{A}} \sim L^{d-1} \log_2 L, \quad (3.4)$$

for both lattice models [103] and continuous fields [102]. The prefactor could only be derived [102] assuming (i) the validity of the Widom conjecture [104] and (ii) its applicability to the functional form of binary entropy. For bosons at criticality, numerical evidence for the area law (3.3) was found for a three-dimensional array of coupled oscillators [108]. Callan and Wilczek derived the area law in approximative field theoretical calculations [109].

Beyond the fundamental physical interest, entanglement scaling sets the scope of numerical methods using tensor contraction ansatz states (see Secs. 1.3–1.5) such as the density-matrix renormalization-group (DMRG) [66, 68], because the computation time required to simulate a quantum state using these methods on classical computers increases exponentially with its entanglement entropy.

In this chapter, the bipartite entanglement entropy is studied in a *unified* treatment for *exactly solvable* two-dimensional fermionic and bosonic models at $T = 0$. To this purpose, the reduced density matrix of a quadratic model is related to its Green's function matrices, generalizing work by Cheong and Henley [172] based on a coherent-state method developed by Chung and Peschel [121]. For the critical fermionic two-dimensional tight-binding model one finds as expected (3.4), but the exact calculation allows to identify the dependence of the scaling law prefactor on the chemical potential μ . This verifies exactly the behavior predicted in [102], where the validity of the Widom conjecture and its applicability to the binary entropy were assumed. Interestingly, one observes a *sublogarithmic* correction to the area law if the gap of the model closes in a zero-dimensional region of momentum space (i.e. one or more points). For a critical bosonic two-dimensional model of coupled harmonic oscillators it is found that the entanglement entropy saturates to the area law (3.4), which confirms [108, 109].

The generic quadratic Hamiltonians studied here are

$$H_{F,B} = \sum_{ij} \left[a_i^\dagger V_{ij} a_j + \frac{1}{2} (a_i^\dagger W_{ij} a_j^\dagger + h.c.) \right], \quad (3.5)$$

where $a_i \equiv c_i$ and $a_i \equiv b_i$ are fermionic and bosonic operators for H_F and H_B respectively. Previous field-theoretical work did not indicate any qualitative dependence of the entanglement entropy scaling on the presence or absence of interactions in the systems. For one-dimensional systems it is known that the decisive difference is the presence or absence of criticality, in whatever way it comes about. This is why the quasi-free case is, for once, highly relevant.

3.1. Calculating entropy from Green's matrices

Let us consider a bipartite universe $\mathcal{AB}$ of N modes (or sites). System $\mathcal{A}$ consists of n sites; in the calculations, eventually, the thermodynamic limit $N \rightarrow \infty$ will be taken. The relation between the Green's function matrices of system $\mathcal{A}$ and its reduced density matrix $\rho_{\mathcal{A}} = \text{Tr}_{\mathcal{B}} \rho$ can be derived by determining the matrix elements of the full density matrix ρ with respect to coherent states and integrating out the variables of the environment $\mathcal{B}$.

3.1.1. Fermionic systems

The Green's function matrix for system $\mathcal{A}$ with respect to the operators $A_i \equiv c_i^\dagger + c_i$ and $B_i \equiv c_i^\dagger - c_i$, as defined by

$$[G_{BA}]_{ij} = \text{Tr} \rho B_i A_j \quad \text{with} \quad i, j \in \mathcal{A}, \quad (3.6)$$

can be obtained *exactly* for the solvable Hamiltonian H_F , Eq. (3.5), following [173]. It can then be shown that $\rho_{\mathcal{A}}$ is given by

$$\langle \xi | \rho_{\mathcal{A}} | \xi' \rangle = \det \left(\frac{\mathbb{1} - G_{BA}}{2} \right) e^{-\frac{1}{2} (\xi^* - \xi')^T \cdot (G_{BA} + \mathbb{1})(G_{BA} - \mathbb{1})^{-1} \cdot (\xi^* + \xi')}, \quad (3.7)$$

where $\xi = (\xi_1 \dots, \xi_n)$ are the Grassmann variables associated with system $\mathcal{A}$, and $|\xi\rangle$ are the corresponding coherent states with $c_i |\xi\rangle = \xi_i |\xi\rangle$. Indeed (3.7) reproduces all two-particle Green's functions correctly and is, due to Wick's theorem, thus the correct reduced density matrix.

To calculate the entropy of system $\mathcal{A}$, we can diagonalize $\rho_{\mathcal{A}}$ by the Bogoliubov transformation

$$f_q = \sum_i \left[\frac{P_{qi} + Q_{qi}}{2} c_i + \frac{P_{qi} - Q_{qi}}{2} c_i^\dagger \right], \quad (3.8)$$

where $PP^T = QQ^T = \mathbb{1}$ (due to the anti-commutation rules), $P_q G_{BA}^T = \nu_q Q_q$ and $Q_q G_{BA} = \nu_q P_q$. The diagonalized reduced density matrix reads

$$\rho_{\mathcal{A}} = \left(\prod_q \frac{1 - \nu_q}{2} \right) \cdot e^{-\sum_q \varepsilon_q f_q^\dagger f_q}, \quad (3.9)$$

with pseudo-energies $\varepsilon_q = \ln \frac{1-\nu_q}{1+\nu_q}$, yielding the entropy

$$S_{\mathcal{A}} = \sum_{q=1}^n h\left(\frac{1+\nu_q}{2}\right), \quad (3.10)$$

with the so-called binary entropy

$$h(x) = -x \log_2 x - (1-x) \log_2 (1-x). \quad (3.11)$$

3.1.2. Bosonic systems

For the quadratic Hamiltonian H_B the Green's function matrices G_{AA} and G_{BB} with respect to the operators $A_i \equiv b_i^\dagger + b_i$ and $B_i \equiv b_i^\dagger - b_i$ can be obtained as in [174]. With respect to the bosonic coherent states $b_i|\phi\rangle = \phi_i|\phi\rangle$, the reduced density matrix then reads

$$\begin{aligned} \langle \phi | \rho_{\mathcal{A}} | \phi' \rangle &= K' e^{\frac{1}{4}(\phi^* + \phi')^T \cdot (G_{AA} - \mathbb{1})(G_{AA} + \mathbb{1})^{-1} \cdot (\phi^* + \phi')} \\ &\quad \times e^{-\frac{1}{4}(\phi^* - \phi')^T \cdot (G_{BB} - \mathbb{1})^{-1}(G_{BB} + \mathbb{1}) \cdot (\phi^* - \phi')}, \end{aligned} \quad (3.12)$$

where $K' = \sqrt{\det(1 + G_{AA})(1 - G_{BB})}$ is determined by the normalization of $\rho_{\mathcal{A}}$.

The Bogoliubov transformation

$$g_q = \sum_i \left[\frac{P_{qi} + Q_{qi}}{2} b_i + \frac{P_{qi} - Q_{qi}}{2} b_i^\dagger \right], \quad (3.13)$$

with $P^T Q = Q^T P = \mathbb{1}$, $P_q G_{AA} = \mu_q Q_q$ and $Q_q G_{BB} = -\mu_q P_q$ diagonalizes $\rho_{\mathcal{A}}$, giving

$$\rho_{\mathcal{A}} = \left(\prod_q \frac{2}{\mu_q + 1} \right) e^{-\sum_q \epsilon_q g_q^\dagger g_q}, \quad (3.14)$$

where $\epsilon_q = \ln \left(\frac{\mu_q + 1}{\mu_q - 1} \right)$ are pseudo-energies. The entropy $S_{\mathcal{A}}$ is the sum of the quasi-particle entropies,

$$S_{\mathcal{A}} = \sum_{q=1}^n \left(\frac{\mu_q + 1}{2} \log_2 \frac{\mu_q + 1}{2} - \frac{\mu_q - 1}{2} \log_2 \frac{\mu_q - 1}{2} \right). \quad (3.15)$$

When choosing $T = 0$, i.e. when ρ is the ground state density matrix, Eq. (3.10) and (3.15) give the entanglement entropy.

3.2. Critical fermionic entanglement and the Widom conjecture

The form of the logarithmic correction to the entanglement entropy in $d > 1$ dimensional critical fermion models and bounds on it have been derived by Wolf [103], Gioev and Klich [102]. Assuming that the Widom conjecture [104] holds also for $d > 1$ and that the non-analyticity of the binary entropy h can be ignored at one point in the calculation, Gioev and Klich [102] arrive at

$$S_{\mathcal{A}} \equiv S_{\Omega}(L) = c(\mu) L \log_2 L + o(L \log_2 L), \quad (3.16)$$

$$c(\mu) = \frac{1}{2\pi} \frac{1}{12} \int_{\partial\Omega} dS_x \int_{\partial\Gamma(\mu)} dS_k |\mathbf{n}_x \cdot \mathbf{n}_k|, \quad (3.17)$$

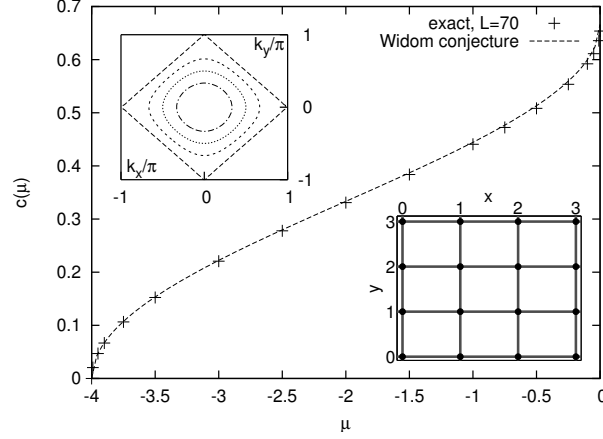


Figure 3.1.: The prefactor $c(\mu)$ in the entanglement entropy scaling law as a function of the chemical potential μ for the ground state of the two-dimensional fermionic tight-binding model in comparison to the result of Gioev and Klich [102]. Insets show the hopping parameters and the Fermi surfaces for $\mu = -3, -2, -1, 0$.

where Ω is the real-space region of $\mathcal{A}$, rescaled by L such that $\text{Vol}(\Omega) = 1$. Vectors $\mathbf{n}_x$ and $\mathbf{n}_k$ denote the normal vectors on the real-space surface $\partial\Omega$ and the Fermi surface $\partial\Gamma(\mu)$. With the method introduced in Section 3.1 applied for $T = 0$, one can calculate the entanglement entropy for finite L *exactly* and thus check (3.16), also shedding some light on the validity of the assumptions leading to (3.17).

3.2.1. Two-dimensional systems with a one-dimensional Fermi surface

The two-dimensional tight-binding model with periodic boundary conditions

$$H = - \sum_{x,y} \left(c_{x,y}^\dagger c_{x+1,y} + c_{x,y}^\dagger c_{x,y+1} + h.c. \right) \quad (3.18)$$

has the dispersion relation

$$E(\mathbf{k}) = -2 \cdot (\cos k_x + \cos k_y). \quad (3.19)$$

The ground state Green's function matrix, from which the entanglement entropy is calculated, reads in the thermodynamic limit

$$G_{\mathbf{r},\mathbf{r}'} = \int_{\Gamma(\mu)} \frac{d^2 k}{(2\pi)^2} e^{i\mathbf{k} \cdot (\mathbf{r} - \mathbf{r}')} , \quad (3.20)$$

with $\mathbf{r} = (x, y)$. Fig. 3.1 shows the scaling prefactor $c(\mu)$ as fitted from the exact entanglement entropy of an $L \times L$ square with the rest of the universe, which was obtained

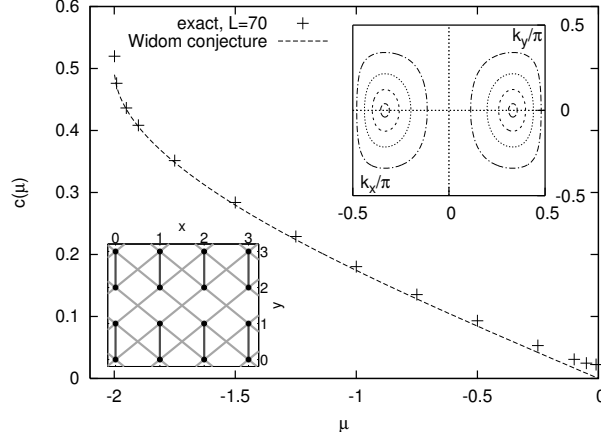


Figure 3.2.: The scaling prefactor $c(\mu)$ for the ground state of a two-dimensional fermionic tight-binding model with next-nearest neighbor hoppings in comparison to the result of [102]. Insets show the hopping parameters and the Fermi surfaces for $\mu \in [-0.25, -1.75]$ in the quartered Brillouin zone.

from (3.10). It is in excellent agreement with (3.17) and supports thus also the Widom conjecture for $d = 2$. The same agreement was found in the model

$$H = - \sum_{x,y} \left((1 + (-1)^y) c_{x,y}^\dagger c_{x,y+1} + c_{x,y}^\dagger c_{x+1,y+1} + c_{x,y}^\dagger c_{x-1,y+1} + h.c. \right) \quad (3.21)$$

which has a two-banded dispersion relation

$$E(\mathbf{k}) = \pm 2 \sqrt{1 + 4 \cos k_x \cos^2 k_y + 4 \cos^2 k_x \cos^2 k_y} \quad (3.22)$$

and a disconnected Fermi surface for $\mu \in [-2, 2]$, Fig. 3.2.

In a later work [106], the correctness of (3.16), (3.17) was in analogous manner also confirmed for a three-dimensional fermionic system.

3.2.2. Two-dimensional systems with a zero-dimensional Fermi surface

Especially for a comparison with bosonic systems, it is interesting to investigate models with a zero-dimensional Fermi surface. In particular the two-dimensional model

$$H = - \sum_{x,y} \left(h \cdot c_{x,y}^\dagger c_{x+1,y} + (1 + (-1)^{x+y}) c_{x,y}^\dagger c_{x,y+1} + h.c. \right), \quad (3.23)$$

is chosen which has for $0 \leq h \leq 1$ the two-band dispersion relation

$$E(\mathbf{k}) = \pm 2 \sqrt{1 + h^2 \cos^2 k_x + 2h \cos k_x \cos k_y}, \quad (3.24)$$

i.e. a gap of size $4(1 - h)$ at $\mathbf{k} = (\pi, 0)$. Fig. 3.3 shows for $\mu = 0$ and $h \rightarrow 1$ how the entanglement entropy converges to the area law with a *sublogarithmic* correction,

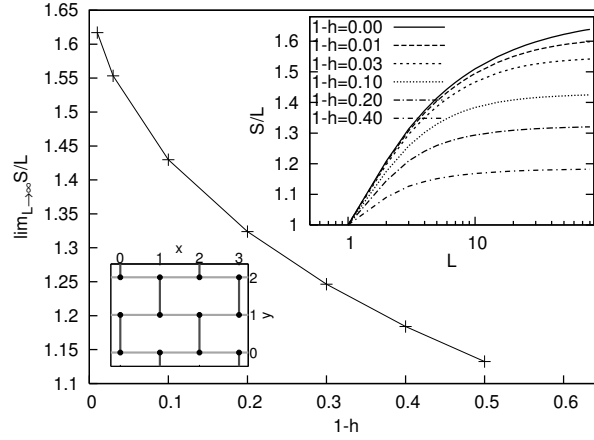


Figure 3.3.: The upper right inset shows the entanglement entropy per surface unit $S_\Omega(L)/L$ (block of $n = L^2$ sites) for a two-dimensional fermionic tight-binding model with modulated vertical hopping (see the second inset) at $T = 0$. The energy gap $4(1 - h)$ closes in the point $\mathbf{k} = (\pi, 0)$. The extrapolation $\lim_{L \rightarrow \infty} S_\Omega(L)/L$ suggests a divergence for $h \rightarrow 1$.

$S_\Omega(L) = L \cdot o(\log_2 L)$, meaning $\lim_{L \rightarrow \infty} S_\Omega(L)/(L \log_2 L) = 0$. The curves $S_\Omega(L)/L$ for finite gaps were extrapolated to obtain $\lim_{L \rightarrow \infty} S_\Omega(L)/L$. Those values indicate indeed a divergence for $h \rightarrow 1$. This result is consistent with Eq. (3.16), as the scaling coefficient $c(\mu)$, Eq. (3.17), vanishes for systems in $d > 1$ dimensions with a zero-dimensional Fermi surface. Further investigations have to determine the analytical form of the sublogarithmic correction and its universality.

3.3. Critical bosonic entanglement

An important question is whether the logarithmic correction observed in the entanglement entropy scaling law for critical one-dimensional bosonic systems is also present in higher dimensional systems. To investigate this, let us examine a two-dimensional system of coupled oscillators

$$H = \frac{1}{2} \sum_{x,y} (\Pi_{x,y}^2 + \omega_0^2 \Phi_{x,y}^2 + (\Phi_{x,y} - \Phi_{x+1,y})^2 + (\Phi_{x,y} - \Phi_{x,y+1})^2), \quad (3.25)$$

where $\Phi_{x,y}$, $\Pi_{x,y}$ and ω_0 are coordinate, momentum and self-frequency of the oscillator at site $\mathbf{r} = (x, y)$. The masses and coupling strengths are set to unity. The system has the dispersion relation

$$E(\mathbf{k}) = \sqrt{\omega_0^2 + 4 \sin^2 k_x/2 + 4 \sin^2 k_y/2}, \quad (3.26)$$

i.e. a gap of size ω_0 at $\mathbf{k} = (0, 0)$.

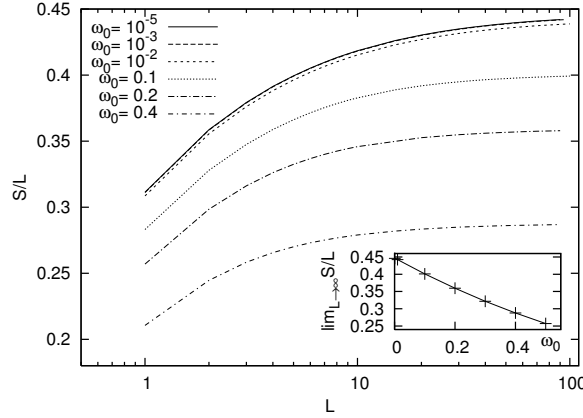


Figure 3.4.: The entanglement entropy per surface unit $S_\Omega(L)/L$ (block with $n = L^2$ sites) for the bosonic two-dimensional system of coupled harmonic oscillators at $T = 0$. The curves converge for small energy gaps ω_0 . The extrapolation $\lim_{L \rightarrow \infty} S_\Omega(L)/L$ yields, for the critical limit, the area law $S_\Omega(L) \approx 0.45 \cdot L$.

In the low-energy limit, the harmonic oscillators can be reduced to a field theory only containing $(\nabla\phi)^2$, which describes a massless free bosonic model. The scaling of entanglement entropy in this model has been studied by Srednicki [108] numerically in $d = 3$ dimensions and by Callan and Wilczek [109] with approximate field theoretical methods for all $d > 1$. Both provide evidence for the area law (3.3).

Applying the transformation

$$b_i = \sqrt{\frac{\omega}{2}} \cdot \left(\Phi_i + \frac{i}{\omega} \Pi_i \right) \quad (3.27)$$

with $\omega = \sqrt{\omega_0^2 + 4}$, the Hamiltonian (3.25) is mapped to the canonical form (3.5) and is thus amenable to the method introduced in Section 3.1. The translation invariant Green's function matrices G_{AA} and G_{BB} of system $\mathcal{A}$ are at $T = 0$

$$G_{AA}(\mathbf{r}, \mathbf{0}) = \frac{1}{\pi^2} \int_0^\pi \int_0^\pi d^2k \frac{\omega}{E(\mathbf{k})} \cos k_x x \cos k_y y$$

$$G_{BB}(\mathbf{r}, \mathbf{0}) = -\frac{1}{\pi^2} \int_0^\pi \int_0^\pi d^2k \frac{E(\mathbf{k})}{\omega} \cos k_x x \cos k_y y$$

and the entanglement entropy is obtained from Eq. (3.15). Special care has to be taken for the limit $\omega_0 \rightarrow 0$, as this results in a singularity of the integrand for G_{AA} . This was done by calculating the entropy for ever smaller but finite gaps ω_0 and refining in each numerical integration the momentum space resolution until the integral converges. The limit $\omega_0 \rightarrow 0$ was then investigated by extrapolation. Fig. 3.4 displays the entanglement entropy as a function of the linear size L of system $\mathcal{A}$ for several ω_0 . The curves converge for $\omega_0 \rightarrow 0$ and a finite-size scaling analysis yields (see the inset) $\lim_{\omega_0 \rightarrow 0} \lim_{L \rightarrow \infty} S_\Omega(L)/L \approx 0.45$,

i.e. the critical model obeys for $d = 2$ the area law $S_{\Omega}(L) \approx 0.45 \cdot L$. The fact that no logarithmic correction is observed although the system is critical may be attributed to the fact that the gap closes in a single point (or zero-dimensional region) of momentum space. This is very similar to the same situation for fermionic systems analyzed in Section 3.2.2.

3.4. Conclusions

A relation between Green's function matrices of quadratic fermionic and bosonic Hamiltonians to reduced density matrices was used to study bipartite entanglement entropy in critical two-dimensional systems. Here, three different regimes for the scaling of the entropy have been identified and substantiated with exact quantitative results:

- For critical fermionic systems with a one-dimensional Fermi surface, it follows the area law with a logarithmic correction and the corresponding prefactor determined in [102] under assumption of the Widom conjecture is correct. This gives also support for the Widom conjecture in two dimensions.
- For critical fermionic systems with a zero-dimensional Fermi surface, it follows the area law with a sub-logarithmic correction.
- For critical bosonic systems, it follows the area law without corrections.

Those findings demonstrate the subtle nature of entanglement at criticality, the physical explanation of which remains a challenging topic for future research.

4. Entanglement entropy beyond the free case for collective models

A perturbative method to compute the ground state entanglement entropy for interacting systems is presented. It is applied to a collective model of mutually interacting spins in a magnetic field. At the quantum critical point, the entanglement entropy scales logarithmically with the subsystem size, the system size, and the anisotropy parameter. The corresponding scaling prefactors and the leading finite-size correction to the entropy are determined. The derived analytical predictions are in perfect agreement with numerical results.

In recent years, much effort has been devoted to the characterization of ground state entanglement in many-particle systems. Especially, its relationship with quantum phase transitions (QPTs) has been investigated, following the seminal works in one-dimensional (1D) systems [135–137]. From these studies several fundamental questions have emerged concerning the universality of the observed behaviors, as well as their classification. For example, the entanglement entropy is known to scale logarithmically with the subsystem size in 1D critical spin chains (see, e.g., Refs. [100, 137, 101, 140] and Sec. 1.4), though its precise form depends on the boundary conditions, cf. [97, 175] and Chap. 2. It is natural to wonder how that behavior is modified in higher-dimensional systems.

To address this question, the Lipkin-Meshkov-Glick model (LMG) [176] of mutually interacting spins in a magnetic field is examined, i.e. a system with an infinite coordination number. Although the model was introduced in nuclear physics, it has been used to describe many other physical systems such as Bose-Einstein condensates [177] or small ferromagnetic particles [178] to cite just a few. Its entanglement properties have been analyzed from different perspectives [179–181], but its entropy has only been studied numerically [182].

The aim of this chapter is to investigate analytically the entanglement entropy in the LMG model. First, the model is studied in the thermodynamic limit for which it can be mapped onto a free bosonic system, allowing for an exact evaluation of the entropy [183, 184, 105]. In a second step, the finite-size corrections to the entropy at and away from the transition point are addressed. This leads to the derivation of a perturbative method, because for a large but finite number of spins, the bosons are weakly interacting. At the critical point, the entropy is found to grow logarithmically with the subsystem size as in the critical 1D XY model [170, 167] which is the 1D counterpart of the LMG model. However, the scaling prefactor differs from the 1D case and also disagrees with previous numerical studies [182]. It is also shown that, at the quantum critical point,

the entropy scales logarithmically with the system size and the anisotropy parameter, and the associated scaling prefactors are computed. Away from criticality, the dependence of the entropy on the subsystem size is found to differ considerably from the scaling in finite-dimensional systems. The validity of the chosen approach is confirmed by numerical exact diagonalization results. Further details are presented in [185].

4.1. Lipkin-Meshkov-Glick model

The LMG model describes the collective behavior of N spins $1/2$ with a mutual anisotropic (XY) ferromagnetic interaction, subjected to an external transverse magnetic field h . The corresponding Hamiltonian H can be expressed in terms of the total spin operators

$$S_\alpha = \sum_i \sigma_\alpha^i / 2, \quad (4.1)$$

where σ_α are the Pauli matrices. Introducing the anisotropy parameter γ , it reads

$$H = -\frac{1}{N} (S_x^2 + \gamma S_y^2) - h S_z. \quad (4.2)$$

Without loss of generality, one can assume $0 \leq \gamma < 1$ and $h \geq 0$. As discussed in the literature, this system undergoes a second-order QPT at $h = 1$, between a symmetric ($h > 1$) and a broken ($h < 1$) phase, which is well described by a mean-field approach. The corresponding classical ground state is fully polarized in the field direction ($\langle \sigma_z^i \rangle = 1$) for $h > 1$, and twofold degenerate with $\langle \sigma_z^i \rangle = h$ for $h < 1$. Entanglement originates from quantum fluctuations around these classical ground states.

4.2. Entanglement entropy

The entanglement entropy in the ground state $|\psi\rangle$ is defined as

$$\mathcal{E} = -\text{Tr}_{\mathcal{A}} (\rho_{\mathcal{A}} \ln \rho_{\mathcal{A}}) = -\text{Tr}_{\mathcal{B}} (\rho_{\mathcal{B}} \ln \rho_{\mathcal{B}}), \quad (4.3)$$

where $\rho_{\mathcal{A},\mathcal{B}} = \text{Tr}_{\mathcal{B},\mathcal{A}} (|\psi\rangle\langle\psi|)$. For practical reasons, $\mathcal{E}$ is defined here with the natural logarithm $\ln$ instead of $\log_2$ as is often done. This definition relies on a splitting of the system into two blocks $\mathcal{A}$ and $\mathcal{B}$, of sizes L and $(N - L)$ respectively. Here, it amounts to introducing

$$S_\alpha^{\mathcal{A},\mathcal{B}} = \sum_{i \in \mathcal{A},\mathcal{B}} \sigma_\alpha^i / 2. \quad (4.4)$$

To describe quantum fluctuations and thus to compute the entanglement entropy, it is convenient to use the Holstein-Primakoff representation of these spin operators [186]

$$S_z^{\mathcal{A}} = L/2 - a^\dagger a, \quad (4.5)$$

$$S_-^{\mathcal{A}} = \sqrt{L} a^\dagger \sqrt{1 - a^\dagger a / L} = (S_+^{\mathcal{A}})^\dagger, \quad (4.6)$$

$$S_z^{\mathcal{B}} = (N - L)/2 - b^\dagger b, \quad (4.7)$$

$$S_-^{\mathcal{B}} = \sqrt{N - L} b^\dagger \sqrt{1 - b^\dagger b / (N - L)} = (S_+^{\mathcal{B}})^\dagger, \quad (4.8)$$

with $S_{\pm}^{\mathcal{A},\mathcal{B}} = S_x^{\mathcal{A},\mathcal{B}} \pm iS_y^{\mathcal{A},\mathcal{B}}$. In this way, the LMG Hamiltonian can be mapped onto a system of two interacting bosonic modes a and b , which satisfy the canonical commutation rules. The above transformation is valid in the symmetric phase, but can also be used in the broken phase, provided one first rotates the z -axis to bring it along the classical spin direction [181].

4.3. Thermodynamic limit

At fixed $\tau = L/N$, the Hamiltonian can be expanded in $1/N$. At order $(1/N)^0$ and for $h > 1$, one gets

$$H = NH^{(-1)} + H^{(0)} + \mathcal{O}(1/N) \quad (4.9)$$

with $H^{(-1)} = -h/2$ and

$$\begin{aligned} H^{(0)} = & -\frac{1+\gamma}{4} + \frac{2h-\gamma-1}{2}(a^\dagger a + b^\dagger b) \\ & + \frac{\gamma-1}{4} \left[\tau(a^{\dagger 2} + a^2) + (1-\tau)(b^{\dagger 2} + b^2) \right. \\ & \left. + 2\sqrt{\tau(1-\tau)}(a^\dagger b^\dagger + ab) \right]. \end{aligned} \quad (4.10)$$

This effective bosonic Hamiltonian for the spin excitations is quadratic, and thus exactly solvable. Following [183, 184], the reduced density matrix can be written as $\rho_{\mathcal{A}} = e^{-K}$ where, at the order considered here, K reads

$$K^{(0)} = \kappa_0^{(0)} + \kappa_1^{(0)} a^\dagger a + \kappa_2^{(0)} (a^{\dagger 2} + a^2). \quad (4.11)$$

The key ingredients leading to this form are: *i*) the eigenvalues of $\rho_{\mathcal{A}}$ are non-negative and smaller than one, which explains the exponential form; *ii*) Wick's theorem holds for quadratic Hamiltonians, constraining $K^{(0)}$ to be quadratic. The three coefficients $\kappa_i^{(0)}$ can be determined from the three conditions

$$\text{Tr}_{\mathcal{A}} \rho_{\mathcal{A}} = 1, \quad \langle\langle a^\dagger a \rangle\rangle = \langle a^\dagger a \rangle \text{ and } \langle\langle a^{\dagger 2} \rangle\rangle = \langle a^{\dagger 2} \rangle, \quad (4.12)$$

where $\langle\Omega\rangle = \langle\psi|\Omega|\psi\rangle$ and $\langle\langle\Omega\rangle\rangle = \text{Tr}_{\mathcal{A}}(e^{-K}\Omega)$. To compute these expectation values, one simply has to diagonalize $H^{(0)}$ and $K^{(0)}$. Then, the $\kappa_i^{(0)}$'s are obtained by solving the 3×3 nonlinear system of equations (4.12). From these coefficients, one finally obtains the entropy [105]

$$\mathcal{E}^{(0)} = \frac{\mu+1}{2} \ln \frac{\mu+1}{2} - \frac{\mu-1}{2} \ln \frac{\mu-1}{2}, \quad (4.13)$$

with $\mu = \alpha^{-1/2} \sqrt{[\tau\alpha + (1-\tau)][\tau + \alpha(1-\tau)]}$, and

$$\alpha = \begin{cases} \sqrt{\frac{h-1}{h-\gamma}} & \text{for } h > 1, \\ \sqrt{\frac{1-h^2}{1-\gamma}} & \text{for } h < 1. \end{cases} \quad (4.14)$$

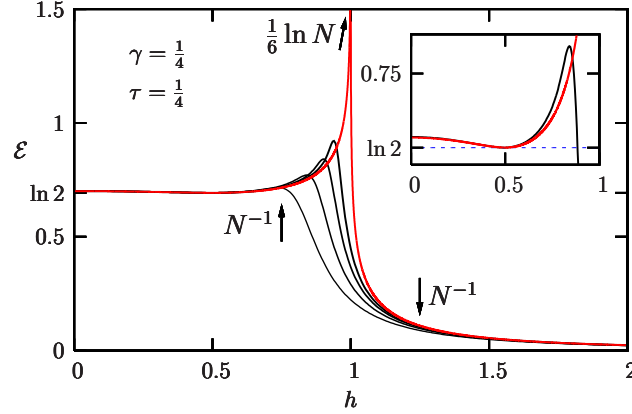


Figure 4.1.: Entanglement entropy as a function of the magnetic field, with fixed $\gamma = 1/4$, $\tau = 1/4$ and $N = 32, 64, 128, 256$ (from numerics) and ∞ ($\mathcal{E}^{(0)}$). Arrows indicate the behavior of the finite-size correction in various regions. For $h < 1$, the figure shows $\mathcal{E}^{(0)} + \ln 2$ for the reason given in the text. The inset is a zoom around $h = \sqrt{\gamma}$ where $\mathcal{E}^{(0)} = 0$, for $N = 64$ (black line) and ∞ (red line).

It is interesting to note that $\alpha = \lim_{N \rightarrow \infty} 4\langle S_y^2 \rangle / N$ also plays an important role for the concurrence which is a two-spin entanglement measure [180, 181].

In the broken phase $h < 1$, the ground state is twofold degenerate in the thermodynamic limit. The two quantum states belong to the maximum spin sector $S = N/2$ and are eigenstates of the spin-flip operator $\prod_i \sigma_z^i$. This degeneracy is lifted for finite N . Here, the entropy stemming from quantum fluctuations around one of the (fully polarized) classical ground states has been calculated. The classical ground states do not coincide with the quantum ground states just discussed. However, they are closely related and it turns out that the difference between $\mathcal{E}^{(0)}$ and the actual entropy is equal to $\ln 2$. Also note that for $h = \sqrt{\gamma}$, the entropy $\mathcal{E}^{(0)}$ vanishes since, there, the two degenerate quantum ground states can be chosen as separable [181].

The comparison of $\mathcal{E}^{(0)}$ with numerical results obtained from exact diagonalization is shown in Fig. 4.1. For large N , excellent agreement is observed in both phases.

4.4. Critical scaling of the entropy

The main characteristic of the entropy $\mathcal{E}^{(0)}$ is that it is finite for $h \neq 1$ whereas it diverges at the critical point, in the vicinity of which one has

$$\begin{aligned} \mathcal{E}^{(0)} = & -\frac{1}{4} \ln |h - 1| + \frac{1}{2} \ln[\tau(1 - \tau)] + \frac{1}{4} \ln(1 - \gamma) + \\ & 1 - x \ln 2 + \mathcal{O}(|h - 1|^{1/2}), \end{aligned} \quad (4.15)$$

with $x = 1$ for $h > 1$ and $x = 5/4$ for $h < 1$. The dependence on h differs from the one given in Ref. [182] where, numerically, the entropy was found to behave as $-\frac{1}{6} \ln |h - 1|$. The discrepancy comes from the too small investigated system sizes as shown in [185]. It is also interesting to note that the same prefactor $-1/4$ was reported in the Dicke model [187] using a different approach and it is very likely shared by a large class of collective models.

As already observed for many physical quantities [180, 181], the $1/N$ expansion of the entropy is singular at the critical point $h = 1$. This is reminiscent of a nontrivial scaling behavior to be discussed in the following. To this purpose let us use the same scaling hypothesis as in Refs. [180, 181] which assumes that in the vicinity of the critical point, a physical observable Φ can be written as the sum of a regular and a singular contribution,

$$\Phi_N(h, \gamma) = \Phi_N^{\text{reg}}(h, \gamma) + \Phi_N^{\text{sing}}(h, \gamma). \quad (4.16)$$

Here, singular means that the function and/or its derivatives with respect to h diverge at the critical point, following a power law. In addition, one has

$$\Phi_N^{\text{sing}}(h \simeq 1, \gamma) \sim \frac{(h - 1)^{\xi_\Phi^h} (1 - \gamma)^{\xi_\Phi^\gamma}}{N^{n_\Phi}} \mathcal{G}_\Phi(\zeta), \quad (4.17)$$

where the scaling variable

$$\zeta = N(h - 1)^{3/2} (1 - \gamma)^{-1/2} \quad (4.18)$$

is introduced. The exponents ξ_Φ^h , ξ_Φ^γ and n_Φ are characteristics of the observables Φ . The behavior of Φ_N^{sing} at the critical point is then obtained by noting that since no divergence can occur at finite N so that one must have

$$\mathcal{G}_\Phi(\zeta) \sim \zeta^{-2\xi_\Phi^h/3} \quad (4.19)$$

and consequently

$$\Phi_N^{\text{sing}}(h = 1, \gamma) \sim N^{-(n_\Phi + 2\xi_\Phi^h/3)} (1 - \gamma)^{\xi_\Phi^\gamma + \xi_\Phi^h/3}. \quad (4.20)$$

To perform such an analysis for the entropy, one is led to consider $\Phi = e^\mathcal{E}$ which, contrary to $\mathcal{E}$, behaves as a power law at lowest order. Combining Eqs. (4.15)-(4.20), one readily identifies $\xi_\Phi^h = -\xi_\Phi^\gamma = -1/4$, and $n_\Phi = 0$. In the large N limit, one thus predicts

$$\mathcal{E}(h = 1) \sim \chi_N \ln N + \chi_\gamma \ln(1 - \gamma) + \chi_\tau \ln[\tau(1 - \tau)], \quad (4.21)$$

with $\chi_N = \chi_\gamma = 1/6$ and $\chi_\tau = 1/2$. This means that, at criticality and for fixed N , the entropy scales as $\frac{1}{2} \ln L$, just like in critical 1D systems. If χ_γ is in agreement with previous numerical results [182], it is not the case for χ_τ which was found to be close to $1/3$.

To check the predictions, a finite-size scaling analysis of these prefactors has been performed. As can be seen in Fig. 4.2, the exponents have not yet reached their asymptotic

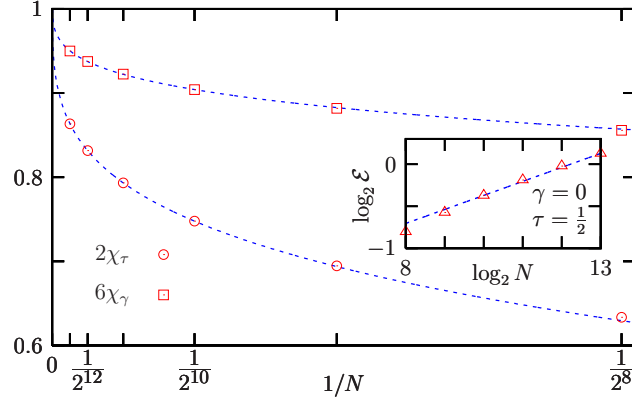


Figure 4.2.: Exponents χ_γ and χ_τ as a function of $1/N$ obtained from numerical diagonalization of H . For clarity, both $2\chi_\tau$ and $6\chi_\gamma$ are plotted which are expected to be equal to 1 in the thermodynamic limit (dotted lines are guides for the eyes). Inset: $\log_2 - \log_2$ plot of the entropy as a function of N at fixed γ and τ . The dotted line has a slope $\chi_N = 1/6$.

value at $N = 2000$ which is the largest size analyzed in Ref. [182]. A simple extrapolation of these finite-size results to the thermodynamic limit confirms the predicted values of χ_N , χ_γ and χ_τ (dotted lines).

As a final word about the values of the prefactors, let us mention that the approach chosen here similarly predicts $\chi_N = 1/6$ in the Dicke model. This is consistent with the value of 0.14 ± 0.01 obtained numerically [187].

4.5. Finite-size corrections

In the following the validity of the scaling hypothesis (4.17) is checked. To this purpose, one must at least compute the $1/N$ correction to the entropy, which requires to develop a perturbation theory to go beyond the free (quadratic) boson case. This calculation will be performed in the symmetric phase only, since this is sufficient to extract the scaling exponents. First of all, one has to expand

$$H = NH^{(-1)} + H^{(0)} + H^{(1)}/N + \mathcal{O}(1/N^2), \quad (4.22)$$

where $H^{(1)}$ is quartic in a and b . The idea is then to expand

$$K = K^{(0)} + K^{(1)}/N + \mathcal{O}(1/N^2), \quad (4.23)$$

with

$$\begin{aligned} K^{(1)} = & \kappa_0^{(1)} + \kappa_1^{(1)} a^\dagger a + \kappa_2^{(1)} (a^{\dagger 2} + a^2) + \kappa_3^{(1)} a^{\dagger 2} a^2 \\ & + \kappa_4^{(1)} (a^{\dagger 3} a + a^\dagger a^3) + \kappa_5^{(1)} (a^{\dagger 4} + a^4). \end{aligned} \quad (4.24)$$

$K^{(1)}$ can not contain any terms of order higher than four in a , because $H^{(0)}$ is quadratic and $H^{(1)}$ quartic in a and b . In the framework of diagrammatic perturbation theory, all terms correspond to certain vertices. Tracing out mode b cannot generate, in $K^{(1)}$, terms of sixth order in a as every effective 6-legged vertex originates from the contraction of at least two bare 4-legged vertices and is thus of order $1/N^2$ or higher. Analogous to the quadratic case, the $\kappa_i^{(1)}$ can be determined from the conditions

$$\begin{aligned} \text{Tr}_{\mathcal{A}} \rho_{\mathcal{A}} &= 1, \quad \langle\langle a^\dagger a \rangle\rangle = \langle a^\dagger a \rangle, \quad \langle\langle a^{\dagger 2} \rangle\rangle = \langle a^{\dagger 2} \rangle, \\ \langle\langle a^{\dagger 2} a^2 \rangle\rangle &= \langle a^{\dagger 2} a^2 \rangle, \quad \langle\langle a^{\dagger 3} a \rangle\rangle = \langle a^{\dagger 3} a \rangle, \quad \langle\langle a^{\dagger 4} \rangle\rangle = \langle a^{\dagger 4} \rangle, \end{aligned} \quad (4.25)$$

which must be satisfied at order $1/N$. These expectation values can be evaluated by diagrammatic perturbation theory. An alternative route, used here, is to compute them by *i*) diagonalizing the quartic operators $H^{(0)} + H^{(1)}/N$ and $K^{(0)} + K^{(1)}/N$ using the canonical transformation method described in Ref. [188] which requires to solve a linear systems of 48 equations for H and of 6 equations for K ; *ii*) solving the 6×6 linear system resulting from (4.25) to obtain the coefficients $\kappa_i^{(1)}$. This second step can be done numerically, but obviously, the full exact solutions of this problem cannot be given explicitly. However, the main interest being the behavior of the entropy near the critical point, its leading contribution has been extracted. It reads

$$\mathcal{E}^{(1)} = -\frac{3(1-\gamma)^{1/2}}{8(h-1)^{3/2}} + \mathcal{O}[(h-1)^{-1}]. \quad (4.26)$$

This correction is in complete agreement with the scaling hypothesis (4.17) since, at this order and in the vicinity of the critical point, one has

$$\begin{aligned} e^{\mathcal{E}} &= e^{\mathcal{E}^{(0)} + \frac{1}{N}\mathcal{E}^{(1)}} \\ &\sim [\tau(1-\tau)]^{1/2} \frac{(1-\gamma)^{1/4}}{(h-1)^{1/4}} \left[1 - \frac{3(1-\gamma)^{1/2}}{8N(h-1)^{3/2}} \right]. \end{aligned} \quad (4.27)$$

As a check for the veracity of this perturbative method, in Fig. 4.3, the numerical and analytical $1/N$ corrections to the entropy are compared as functions of h . For increasing N , the numerical corrections converge quickly towards the analytical one. The inset is a check of the Taylor expansion (4.26) in the vicinity of the critical point.

The scaling (4.21) of the entanglement entropy has to be compared to results obtained for other critical spin systems. In 1D, the entropy at the critical point also scales logarithmically with the subsystem size L with a prefactor depending on the universality class [137]. For example, in the XY model in a transverse field, the entropy obeys a scaling law similar to (4.21) but with differing prefactors [170, 167]. Away from criticality, the entropy of typical finite-dimensional systems is, on scales greater than the correlation length, proportional to the surface area of the considered subsystem. (At criticality, logarithmic corrections can occur [109, 103, 102, 105, 106].) Non-critical collective models however behave differently, due to their infinite coordination number. In particular, the expansion of (4.13) for $h \neq 1$ and small $\tau = L/N$ yields the scaling $\mathcal{E}^{(0)} \propto -\tau \ln \tau + \mathcal{O}(\tau)$.

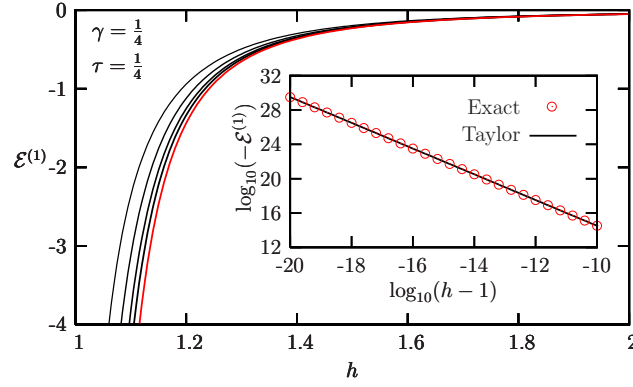


Figure 4.3.: Behavior of $N[\mathcal{E}_{\text{num}} - \mathcal{E}^{(0)}]$ as a function of h for fixed $\tau = 1/4$ and $N = 32, 64, 128, 256$ (from numerics [black lines]) and ∞ ($\mathcal{E}^{(1)}$ obtained from the perturbative expansion [red lines]). Inset: Comparison between $\mathcal{E}^{(1)}$ (dots) and its Taylor expansion (4.26) (solid line).

It should be emphasized that the perturbation theory developed here and applied to the LMG model should not be associated to this model. It may be extended to more complex systems, provided one is able to determine $K^{(1)}$.

5. Dephasing, the steady state, and its entanglement entropy for integrable systems

Here, the relaxation in bosonic and fermionic many-particle systems is addressed. For integrable systems, the time evolution can cause a dephasing effect, leading for finite subsystems to certain steady states. An explicit derivation of those steady subsystem states is given and sufficient prerequisites are devised under which the dephasing takes place. Also simple scenarios are presented, in which dephasing is ineffective and the dependence on dimensionality and criticality is discussed. It follows further that, after a quench of system parameters, bipartite entanglement entropy will become extensive. This provides a way of creating strong entanglement in a controlled fashion, and hinders, on the other hand, the efficient simulation of time evolution via tensor contraction ansatz states for long times.

In equilibrium statistical physics we usually work with canonical ensembles, characterized by density matrices

$$\hat{\rho} \propto e^{-\sum_k \alpha_k \hat{O}_k} \quad (5.1)$$

that can be derived by maximizing the entropy under the constraint of fixed expectation values $\langle \hat{O}_k \rangle$ for a few (macroscopic) observables like energy or particle number [189]. However, it is in general unclear whether a given system in a certain initial state will evolve to any steady state at all and if so, whether that state is indeed one of the canonical ensembles. Recent experiments, especially with ultracold gases, have revived the interest in this important topic of nonequilibrium physics. In such experiments with integrable systems, absence of thermalization was observed (e.g., in [190]). Here it will be deduced analytically under what circumstances integrable systems relax to non-canonical steady states.

It was conjectured in [191] that the time evolution in an integrable system with conserved observables $\hat{I}_k$ should lead to the corresponding maximum entropy ensemble [189]

$$\tilde{\rho}_d = \frac{1}{Z} e^{-\sum_k \alpha_k \hat{I}_k}, \quad (5.2)$$

where the α_k are determined by the initial state. So far, the conjecture was discussed by analyzing specific observables for specific systems [191–194]. In [195] it was found that certain observables do not relax to the ones predicted by the ensemble $\tilde{\rho}_d$ as conjectured in [191]. So here the focus will be not on observables but states themselves.

It is essential, for the conjecture to hold, to restrict oneself to measurements in a finite subsystem, i.e. (5.2) should not be interpreted as the steady state of the full system (see a first discussion in [196]). A general proof is given, showing explicitly how state relaxation in such subsystems can occur due to dephasing. The necessary prerequisites are devised, the relaxation speed is discussed, and simple examples and counter examples for dephasing are given. The results allow for a simple interpretation of the discrepancies between [191] and [195]. On general grounds it follows further that through dephasing the bipartite entanglement entropy in a pure state will become extensive. This may be of interest for quantum computation applications where entanglement is needed as a resource. It has also implications for the ability to simulate such systems on classical computers. The chapter begins with the treatment of free systems, it is then pointed out how this could be generalized to Bethe Ansatz integrable models and the chapter closes with a short discussion of nonintegrable systems.

5.1. Dephasing for quadratic Hamiltonians

Let us first address the situation of quadratic Hamiltonians (for $t > 0$),

$$\hat{H} = \sum_{ij} [a_i^\dagger V_{ij} a_j + \frac{1}{2}(a_i^\dagger W_{ij} a_j^\dagger + h.c.)] + const., \quad (5.3)$$

where a_i are bosonic or fermionic ($\zeta := \pm 1$) ladder operators,

$$[a_i, a_j^\dagger]_{-\zeta} = \delta_{ij} \quad \text{and} \quad \mathbf{a}^\top := (a_1, a_2, \dots). \quad (5.4)$$

This covers also lattice regularized free field theories. The Hamiltonian is diagonalized by a linear canonical transformation

$$\begin{pmatrix} \mathbf{a} \\ \mathbf{a}^\dagger \end{pmatrix} = U \begin{pmatrix} \boldsymbol{\eta} \\ \boldsymbol{\eta}^\dagger \end{pmatrix}, \quad \hat{H} = (\boldsymbol{\eta}^\dagger)^\top \varepsilon \boldsymbol{\eta} = \sum_k \varepsilon_k \eta_k^\dagger \eta_k, \quad (5.5)$$

where ε is the diagonal matrix of one-particle energies. For quadratic systems, the ground state, thermal or evolved states are all Gaussian. Assuming such a Gaussian initial state $\hat{\rho}_{t=0}$, due to the Wick theorem, the state is always fully characterized by the one-particle Green's functions $\mathcal{G}$ (superscripts a, η indicate the chosen one-particle basis)

$$\hat{\rho} = \hat{\rho}(\mathcal{G}), \quad \mathcal{G}^a \equiv \left\langle \begin{pmatrix} \mathbf{a} \\ \mathbf{a}^\dagger \end{pmatrix} \cdot \begin{pmatrix} \mathbf{a}^\dagger \\ \mathbf{a} \end{pmatrix}^\top \right\rangle_{\hat{\rho}} = U \mathcal{G}^\eta U^\dagger. \quad (5.6)$$

The initial state $\hat{\rho}_0$ might, e.g., be the ground state of a different quadratic Hamiltonian (“quench” of system parameters at $t = 0$). In the following, bipartitions of the full system into a subsystem Ω and its environment $\Omega^\perp$ are considered. The projection onto Ω is denoted by Θ_Ω , and the volume by $\mathcal{V} := \text{Vol } \Omega + \text{Vol } \Omega^\perp$. In the situation where $\Omega^\perp$ is approaching the thermodynamic limit, the quantum number labels k become a set of

d continuous labels and one discrete label $k \rightarrow (\mathbf{k}, s)$ (e.g., a d -dimensional momentum vector and a band index, $\varepsilon_k = \varepsilon_{\mathbf{k}s}$ denoting the dispersion relation) with $\mathbf{k} \in \Gamma$, $\text{Vol } \Gamma$ finite, and the density of states $\rho_s \propto 1/\mathcal{V}$. Again, due to the Wick theorem, reduced density matrices $\text{Tr}_{\Omega^\perp} \hat{\rho}$ of quadratic systems are functions of the one-particle subsystem Green's functions G , i.e. $\text{Tr}_{\Omega^\perp} \hat{\rho} = \hat{\rho}(G)$, where G is defined by

$$G^a := \Theta_\Omega \mathcal{G}^a \Theta_\Omega^\top \quad (5.7)$$

with the projection

$$[\Theta_\Omega]_{i,j} = \delta_{i,j} \quad \forall_{i \in \Omega, j \in \Omega \cup \Omega^\perp} \quad (5.8)$$

onto the subsystem Ω .

5.1.1. Theorem

Let the Green's function $\mathcal{G}_d$ be defined by

$$[\mathcal{G}_d^\eta]_{kk'} := \delta_{kk'} [\mathcal{G}_{t=0}^\eta]_{kk}, \quad (5.9)$$

i.e., in the eigenbasis representation, $\mathcal{G}_d$ is the diagonal part of the initial state Green's function $\mathcal{G}_{t=0}$. Under preconditions (a-c), stated after the proof in Sec. 5.1.3, the steady $t \rightarrow \infty$ state of the subsystem Ω is then given by

$$\lim_{t \rightarrow \infty} \text{Tr}_{\Omega^\perp} \hat{\rho}_t = \text{Tr}_{\Omega^\perp} \hat{\rho}_d \quad \text{with} \quad \text{Tr}_{\Omega^\perp} \hat{\rho}_d = \hat{\rho}(G_d), \quad (5.10)$$

i.e. subsystem states relax to the reduced density matrices of $\hat{\rho}_d = \tilde{\rho}_d$, the maximum entropy ensemble (5.2) with

$$\hat{I}_k = \eta_k^\dagger \eta_k \quad \text{and} \quad \alpha_k = \ln(\zeta / (1 - [\mathcal{G}_d^\eta]_{kk}^{-1})). \quad (5.11)$$

5.1.2. Proof

To compare the two reduced density matrices in proposition (5.10), we can first compare the corresponding subsystem Green's functions. That is, instead of addressing (5.10) directly, it is analyzed first under what preconditions the Green's function version

$$\lim_{t \rightarrow \infty} G_t = G_d \quad (5.12)$$

of the theorem is true. Those Green's functions can be expressed as

$$G_d^a = \Theta_\Omega (U \mathcal{G}_d^\eta U^\dagger) \Theta_\Omega^\top, \quad \text{and} \quad (5.13)$$

$$G_t^a = \Theta_\Omega \langle \hat{u}_t^\dagger \left(\begin{smallmatrix} \mathbf{a} \\ \mathbf{a}^\dagger \end{smallmatrix} \right) \left(\begin{smallmatrix} \mathbf{a}^\dagger \\ \mathbf{a} \end{smallmatrix} \right)^\top \hat{u}_t \rangle_{\hat{\rho}_0} \Theta_\Omega^\top = \Theta_\Omega U u_t^\eta \mathcal{G}_0^\eta (u_t^\eta)^\dagger U^\dagger \Theta_\Omega^\top, \quad (5.14)$$

where $\hat{u}_t = e^{\hat{H}t/i\hbar}$, $u_t^\eta = e^{\mathcal{E}t/i\hbar}$, and $\mathcal{E} := \begin{pmatrix} \varepsilon & \\ & -\varepsilon \end{pmatrix}$. Hence, the time-evolved subsystem Green's function G_t^a is of the form

$$G_t^a = \frac{1}{\mathcal{V}} \sum_{kk'} e^{(\mathcal{E}_k - \mathcal{E}_{k'})t/i\hbar} f_{kk'}, \quad \text{with} \quad (5.15)$$

$$f_{kk'} := \mathcal{V} \cdot \Theta_\Omega \mathbf{U}_k [\mathcal{G}_0^\eta]_{kk'} \mathbf{U}_{k'}^\dagger \Theta_\Omega^\dagger, \quad (5.16)$$

where $\mathbf{U}_k$ are the one-particle eigenstates with $[\mathbf{U}_k]_i := U_{ik}$, as introduced in Eq. (5.5). The integrand $f_{kk'}$ in Eq. (5.16) is a matrix valued function of k and k' , whose matrix indices label points in Ω .

The comparison of G_t^a , Eq. (5.15), to G_d^a , Eq. (5.13), tells us that the Green's function version (5.12) of the theorem is true, if the nondiagonal contributions to G_t^a , $k \neq k'$ in the sum of Eq. (5.15), vanish for $t \rightarrow \infty$. The summation over k , for a fixed $\Delta k = k - k' \neq 0$, corresponds for increasing t to a Fourier transform with respect to ever higher frequencies which may vanish due to phase averaging (hence let us call the effect “dephasing”): To see this, we can rewrite G_t^a , Eq. (5.15), with $(k, k') \mapsto (\mathbf{k}, s, \mathbf{k}' = \mathbf{k} + \Delta \mathbf{k}, s')$ as¹

$$G_t^a \rightarrow \sum_{ss'} \frac{1}{\mathcal{V} \rho_s} \sum_{\Delta \mathbf{k}} \int d^d k e^{-i\varphi_{\Delta \mathbf{k}}^{ss'}(\mathbf{k})t} f_{\Delta \mathbf{k}}^{ss'}(\mathbf{k}), \quad (5.17)$$

with phase function φ and group velocity difference $\mathbf{g}$ defined as

$$\varphi_{\Delta \mathbf{k}}^{ss'}(\mathbf{k}) := \frac{\mathcal{E}_{\mathbf{k}s} - \mathcal{E}_{(\mathbf{k}+\Delta \mathbf{k})s'}}{\hbar} \quad \text{and} \quad \mathbf{g}_{\Delta \mathbf{k}}^{ss'}(\mathbf{k}) := \partial_{\mathbf{k}} \varphi_{\Delta \mathbf{k}}^{ss'}(\mathbf{k}). \quad (5.18)$$

In the following, indices s, s' , and $\Delta \mathbf{k}$ are suppressed, and everywhere nondiagonal contributions to (5.17) are considered, i.e. $s \neq s'$ or $\Delta \mathbf{k} \neq \mathbf{0}$. If φ is continuously differentiable, i.e. $\varphi \in \mathcal{C}^1$, $\mathbf{g}$ is finite on the support $\text{supp}(f) \subset \Gamma$ of f , and if the matrix elements of f are $\mathcal{L}^1$ integrable², the integral of (5.17) vanishes for $t \rightarrow \infty$ according to the Riemann-Lebesgue Lemma. This is due to the fast oscillation of the Fourier kernel $e^{-i\mathbf{g} \cdot (\mathbf{k} - \mathbf{k}_0)t}$ in the vicinity of every point $\mathbf{k}_0$. Further, if the amplitude f is bounded in a vicinity $\mathcal{B}$ of $\mathbf{k}_0$, the contribution of $\mathcal{B}$ to the integral is of $\mathcal{O}(\text{Vol } \mathcal{B}/t)$, i.e. vanishes at least as $1/t$.

But what happens at points $\mathbf{k}_0$ where $\mathbf{g}$, the difference of group velocities (5.18), vanishes? If such a zero of $\mathbf{g}$, is isolated, i.e. if the Hesse matrix of φ at $\mathbf{k}_0$ is invertible, and if the amplitude f is smooth in a vicinity of $\mathbf{k}_0$, its contribution to the integral in Eq. (5.17) is still vanishing. This follows from the Morse lemma and a Gaussian integral. We can also treat the case where the Hesse matrix

$$\mathfrak{H}_\varphi := \frac{\partial}{\partial \mathbf{k}} \left(\frac{\partial}{\partial \mathbf{k}} \right)^\top \varphi|_{\mathbf{k}_0} =: W^\top h W \quad (5.19)$$

has only n ($1 \leq n \leq d$) nonzero eigenvalues $\{h_i\}_{1 \leq i \leq n}$. With the coordinate transformations

$$\mathcal{M}_1 : \mathbf{k} \mapsto (\mathbf{q}', \mathbf{q}'') := \mathbf{q} = W \cdot (\mathbf{k} - \mathbf{k}_0), \quad (5.20)$$

¹One needs to exclude cases where single modes give, in the thermodynamic limit, finite contributions to the sum.

² $f \in \mathcal{L}^1$ means that $\int d^d k |[f(\mathbf{k})]_{ij}|$ exists $\forall_{ij}$.

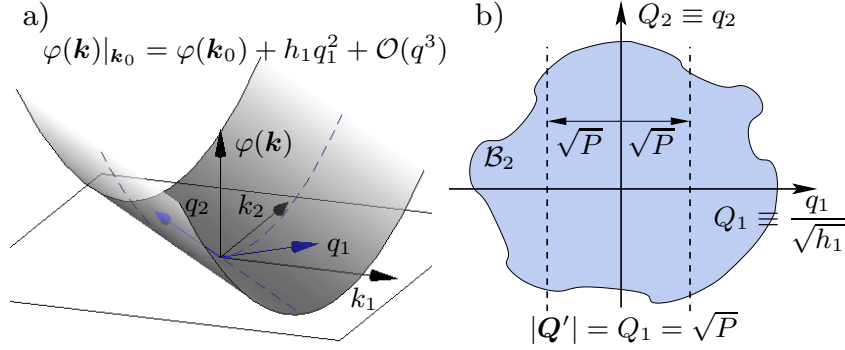


Figure 5.1.: Sketch of (a) the coordinate transformation for Eq. (5.22) and (b) the integration path in Eq. (5.25) for a non-isolated zero of the difference $\mathbf{g}$ of group velocities, Eq. (5.18), in $d = 2$ dimensions and with $n = 1$ nonzero eigenvalues of the Hesse matrix (5.19).

where $\mathbf{q}' \in \mathbb{R}^n$, $\mathbf{q}'' \in \mathbb{R}^{d-n}$, and

$$\mathcal{M}_2 : \mathbf{q} \mapsto (\mathbf{Q}', \mathbf{Q}'') = (h^{-1/2} \mathbf{q}', \mathbf{q}''), \quad (5.21)$$

the contribution from a vicinity $\mathcal{B}$ of $\mathbf{k}_0$ becomes (see Fig. 5.1)

$$\begin{aligned} \int_{\mathcal{B}} d^d k e^{-i\varphi(\mathbf{k})t} f(\mathbf{k}) &= \int_{\mathcal{B}_2} d^d Q e^{-it \sum Q_i'^2 + \mathcal{O}(Q^3)} f_2(\mathbf{Q}) \\ &\sim \int dP e^{-itP} F(P), \end{aligned} \quad (5.22)$$

where

$$\mathcal{B}_2 \equiv \mathcal{M}_2(\mathcal{M}_1(\mathcal{B})), \quad (5.23)$$

$$f_2 \equiv f \circ \mathcal{M}_1^{-1} \circ \mathcal{M}_2^{-1}, \text{ and} \quad (5.24)$$

$$F(P) := \frac{1}{2\sqrt{P}} \int_{\mathcal{B}_2, |Q'|=\sqrt{P}} d^{d-1} Q f_2(\mathbf{Q}). \quad (5.25)$$

See Fig. 5.1 for an illustrative example of the considered coordinate transformations and the integration contour in Eq. (5.25). Integral (5.22) has again the form of a Fourier transform and vanishes for $t \rightarrow \infty$, if $F \in \mathcal{L}^1(\mathcal{B}_2)$. If F is bounded in the vicinity of $P = 0$, the integral vanishes as $\mathcal{O}(\text{Vol } \mathcal{B}/t)$. Those conditions on F have to be interpreted as stricter conditions on the amplitude f when approaching zeros of $\mathbf{g}$, appropriate to still guarantee the dephasing. Zeros of $\mathbf{g}$ with multiplicity $\ell - 1 > 0$ (i.e. $\mathfrak{H}_\varphi = 0$) can be treated in a general fashion only for the case of $d = 1$ dimensions by substituting $Q = q^\ell$. In higher dimensions they are a lot more complicated; see, e.g., [197] for the two-dimensional case.

5. Dephasing, the steady state, and its entanglement entropy for integrable systems

In the cases discussed so far, it was assumed that φ is continuously differentiable ($\varphi \in \mathcal{C}^1$). For the sake of brevity let us now only consider the scenario

$$\varphi(\mathbf{k}) = \varphi_0 + |\mathbf{k}|^\ell + \mathcal{O}(k^{\ell+1}). \quad (5.26)$$

This is for $\ell = 1$ nondifferentiable. The cases $\ell = 1$ and $\ell = 2$ cover very typical examples (for example the linear or quadratic dispersion relations of magnons, phonons, or free particles). The contribution of a (small) sphere of radius K around $\mathbf{k}_0 = \mathbf{0}$ to the integral in (5.17) is with the substitution $P = k^\ell$

$$\approx \int_0^{K^\ell} dP e^{i(\varphi_0 + P)t} \tilde{F}(P), \quad \tilde{F}(P) := \frac{P^{\frac{1-\ell}{\ell}}}{\ell} \int_{|\mathbf{k}|=P^{\frac{1}{\ell}}} d^{d-1}k f(\mathbf{k}). \quad (5.27)$$

This contribution vanishes for $t \rightarrow \infty$ if $\tilde{F} \in \mathcal{L}_{loc}^1$ and if $\tilde{F}$ is bounded, the contribution is of $\mathcal{O}(K^d/t)$.

So far, for a few general, physically relevant scenarios, sufficient conditions have been established under which (every matrix element of) the integral in (5.17) goes to zero as $t \rightarrow \infty$. As $\text{Vol } \Gamma$ is finite and as we have a finite number of bands s , those conditions guarantee hence that all nondiagonal contributions to G_t^a vanish. The Green's function version (5.12) of the theorem is then true. Due to Wick's theorem, expectation values of arbitrary observables $\hat{O}$ on Ω are given by polynomials in $[G_t^a]_{ij}$. Nondiagonal contributions to $\langle \hat{O} \rangle$ will consequently also vanish if we restrict to finite subsystem sizes $\text{Vol } \Omega$. From the convergence $G_t^a \rightarrow G_d^a$ follows then the proposition (5.10). Finally, (5.11) follows from $\langle \eta_k^\dagger \eta_k \rangle_{\tilde{\partial}_d} = 1/(e^{\alpha_k} - \zeta)$ and $\zeta \langle \eta_k^\dagger \eta_k \rangle_{\hat{\partial}_d} = [\mathcal{G}_d^\eta]_{kk} - 1$. $\square$

5.1.3. Preconditions

During the proof, the following prerequisites were collected that are sufficient to guarantee convergence to the steady state (5.10):

- (a) $\text{Vol } \Omega$ is finite and $\mathcal{V} \rightarrow \infty$.
- (b) The parametrization $k \rightarrow (\mathbf{k} \in \Gamma, s)$ of the quantum numbers is possible with a finite $\text{Vol } \Gamma$ and a finite number of bands s .
- (c.1) $\varphi \in \mathcal{C}^1$, g finite on $\text{supp } f \subset \Gamma$, and $f \in \mathcal{L}^1$. If this is not given for the vicinity of a point $\mathbf{k}_0$, we require for such a point
- (c.2) if $g(\mathbf{k}_0) = \mathbf{0}$, then the Hesse matrix $\mathcal{H}_\varphi|_{\mathbf{k}_0}$, Eq. (5.19), exists and is nonzero, and $F \in \mathcal{L}^1$ [Eq. (5.25)], or
- (c.3) if, at $\mathbf{k}_0 = \mathbf{0}$, $\varphi(\mathbf{k}) = \varphi_0 + |\mathbf{k}|^\ell + \mathcal{O}(k^{\ell+1})$ then $\tilde{F} \in \mathcal{L}^1$ [Eq. (5.27)].

Of course, (c.3) can be generalized to the case $|\mathbf{k}|^\ell \rightarrow |A \cdot (\mathbf{k} - \mathbf{k}_0)|^\ell$ with some nonzero matrix A .

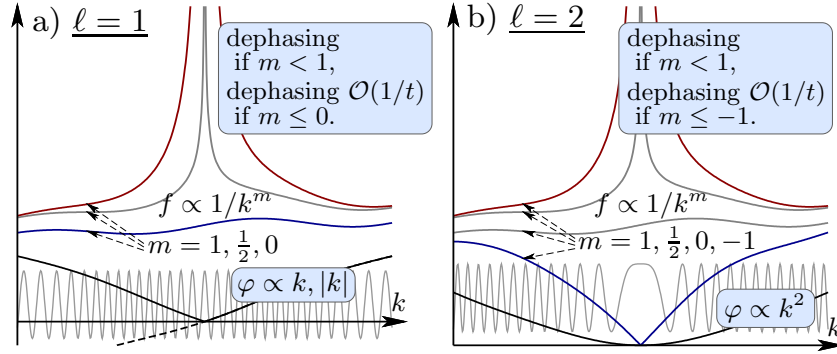


Figure 5.2.: Phase function φ , $\sin(\varphi(k)t)$, and the nondiagonal contribution f to G_t^a in the paradigmatic case (5.29) for $d = 1$ dimensions. As follows from Eq. (5.30), for both, linear dispersion (a), or quadratic dispersion (b) of g , dephasing occurs if $m < 1$, i.e. if f diverges slower than $1/k$. Dephasing occurs as $\mathcal{O}(1/t)$, for the linear dispersion if $m \leq 0$ (no divergence), or $m \leq -1$ ($f(k) \sim k$) for the quadratic dispersion.

With those conditions, all nondiagonal contributions to the subsystem Green's function matrix G_t^a vanish for $t \rightarrow \infty$ and dephasing to the steady state ensemble is effective, (5.10). If f , F , and $\tilde{F}$ are, in the corresponding situations, bounded instead of only $\mathcal{L}^1$ integrable, nondiagonal contributions to G_t^a decay (more quickly) as $\mathcal{O}(1/t)$. Below, illustrative examples are given. Among those are simple scenarios where some of the prerequisites are violated and dephasing does in fact not occur.

5.2. Examples and counter-examples for dephasing

5.2.1. Finite subsystem size $\text{Vol } \Omega$

At the end of the proof, a reason for requiring (in the thermodynamic limit) a finite subsystem size $\text{Vol } \Omega$, precondition (a), was given. A simple counter-example consists in violating precondition (a) by choosing $\Omega^\perp = \emptyset$ and measuring correlators between eigenmodes

$$\zeta \langle \eta_{k'}^\dagger \eta_k \rangle_{\hat{\Omega}_t} = e^{-i\varphi_{kk'}t} [\mathcal{G}_0^\eta]_{kk'} - \delta_{kk'}. \quad (5.28)$$

This expectation value is for all times oscillating; i.e. measurements in infinite subsystems, can reveal the phases and nondiagonal contributions ("rephasing").

5.2.2. Paradigmatic example for zeros of g or divergences of f

If g has zeros or if the amplitude f has divergences, dephasing properties are dominated by the vicinities of such points. Thus, one can illustrate precondition (c) by considering

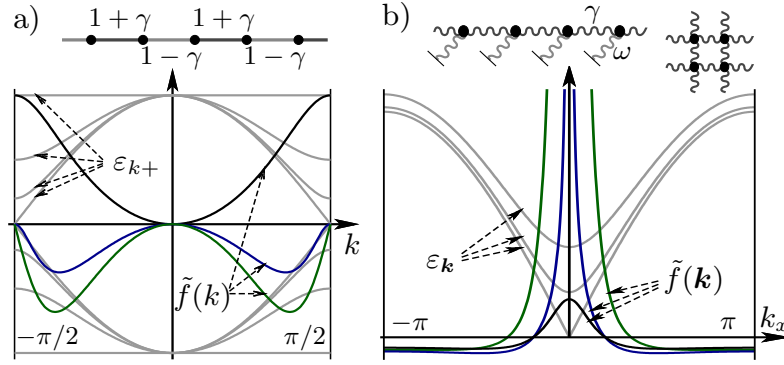


Figure 5.3.: a) One-dimensional fermionic dimerized tight-binding model (5.31). Dispersion relation $\varepsilon_{k\pm} = \mp\varphi(k)/2$ for $\gamma = 1, \frac{1}{2}, \frac{1}{5}, 0$ and the nondiagonal contribution $\tilde{f}(k)$ to $\langle c_1 c_0^\dagger \rangle_t$ according to Eq. (5.33) for quenches $\gamma = \frac{1}{2} \rightarrow 0, \frac{1}{5} \rightarrow \frac{1}{2}, 0 \rightarrow \frac{1}{2}$ (top to bottom). b) The d -dimensional harmonic lattice model. Dispersion relation $\varepsilon_{\mathbf{k}} = -\varphi(\mathbf{k})/2$ for $\omega = \frac{4}{5}, \frac{2}{5}, 0$ with $\gamma = 1$, and the nondiagonal contribution $\tilde{f}(\mathbf{k})$ to $\langle b_{\mathbf{x}} b_{\mathbf{x}'}^\dagger \rangle_t$ according to Eq. (5.36) for quenches $\omega = \frac{4}{5} \rightarrow 0, 0 \rightarrow \frac{4}{5}, \frac{2}{5} \rightarrow \frac{4}{5}$ (top to bottom).

the paradigmatic scenario

$$\varphi(\mathbf{k}) \sim \varphi_0 + |\mathbf{k}|^\ell, \quad f(\mathbf{k}) \sim 1/k^m \quad \text{near } \mathbf{k} = \mathbf{0} \quad (5.29)$$

(for some fixed $s, s', \Delta\mathbf{k}$ and fixed matrix indices $i, j \in \Omega$). The integral in (5.17) is then

$$e^{i\varphi_0 t} \int d^d k \frac{1}{|\mathbf{k}|^m} e^{i|\mathbf{k}|^\ell t} \sim \int dq \frac{1}{q^\chi} e^{iqt}, \quad \chi = \frac{m + \ell - d}{\ell}. \quad (5.30)$$

Hence this (nondiagonal) contribution to G_t^a , for $t \rightarrow \infty$,

- does not vanish if $\chi \geq 1$,
- vanishes as $1/t^{1-\chi}$ if $0 < \chi < 1$,
- and (at least) as $1/t$ if $\chi \leq 0$;

see Fig. 5.2. In this scenario, both preconditions (c.2) and (c.3) apply with $F, \tilde{F} \propto P^{-\chi}$ and are not only sufficient but also necessary.

5.2.3. One-dimensional fermionic dimerized tight-binding model

The first explicit example is ($a_i \equiv c_x, \hbar = 1$)

$$\hat{H} = - \sum_x (1 + \gamma(-1)^x) [c_x^\dagger c_{x+1} + h.c.], \quad (5.31)$$

the dimerized fermionic tight-binding model, where modes c_k and $c_{k+\pi}$ are coupled and the dispersion relation is

$$\varepsilon_{k\pm} = \pm 2\sqrt{\cos^2 k + \gamma^2 \sin^2 k}, \quad (5.32)$$

i.e. gapless if $\gamma = 0$. The eigenmodes are labeled $\eta_{k\pm}$. The ground state for a certain dimerization γ_0 is evolved with a different value $\gamma \neq \gamma_0$ for some time t . Details of the calculation are skipped here. Using Eq. (5.17), the nondiagonal contributions $\langle c_x c_{x'}^\dagger \rangle_t^{nd}$ from $\langle \eta_{k+} \eta_{k-}^\dagger \rangle$ and $\langle \eta_{k-} \eta_{k+}^\dagger \rangle$ to $\langle c_x c_{x'}^\dagger \rangle_t$ can be written as

$$\langle c_x c_{x'}^\dagger \rangle_t^{nd} = \int_0^{\frac{\pi}{2}} dk \tilde{f}(k) \cdot \begin{cases} \cos(\varphi(k)t), & \text{odd } x - x' \\ i \sin(\varphi(k)t), & \text{even } x - x' \end{cases} \quad (5.33)$$

Fig. 5.3a displays $\varepsilon_{k\pm} = \mp \varphi(k)/2$ and $\tilde{f}$ for $(x, x') = (1, 0)$ and three different quenches with $\gamma \neq 1$. The zeros of g are $k = 0, \pm \frac{\pi}{2}$ and have each, in the notation of the paradigmatic situation (5.29), one of the characteristics $(\ell, m) = (2, -2), (1, 0), (2, -1)$. Hence, $\chi < 0$ and dephasing of $\mathcal{O}(1/t)$ is guaranteed. The same is given for all other (x, x') and has also been checked numerically. However, if one switches to $\gamma = 1$, φ has the constant value -4 for all k and no dephasing can occur – we have uncoupled dimers.

5.2.4. Harmonic lattice model

As a second explicit example let us consider the harmonic lattice model in d dimensions, i.e. a lattice of coupled quantum mechanical harmonic oscillators ($a_i \equiv b_{\mathbf{r}}, \hbar = 1$). Contrary to the first example, it will not dephase in all cases.

$$\hat{H} = \frac{1}{2} \sum_{\mathbf{r}} [P_{\mathbf{r}}^2 + \omega^2 Q_{\mathbf{r}}^2 + \gamma \sum_{i=1}^d (Q_{\mathbf{r}} - Q_{\mathbf{r}+\mathbf{e}_i})^2]. \quad (5.34)$$

The dispersion relation is

$$\varepsilon_{\mathbf{k}} = \sqrt{\omega^2 + 4\gamma \sum_{i=1}^d \sin^2 k_i/2}, \quad (5.35)$$

i.e. gapless for $\omega = 0$. With the bosonic operators $b_{\mathbf{r}} := (Q_{\mathbf{r}} + iP_{\mathbf{r}})/\sqrt{2}$, the Hamiltonian $\hat{H}$ is brought to the form (5.3) and is hence amenable to the theorem. Using (5.17) one arrives at

$$\begin{aligned} \langle b_{\mathbf{r}} b_{\mathbf{r}'}^\dagger \rangle_t^{nd} &= \int_{-\pi}^{\pi} d^d k f(\mathbf{k}) \cos(2\varepsilon_{\mathbf{k}} t), \quad f = e^{i\mathbf{k} \cdot (\mathbf{r} - \mathbf{r}')} \tilde{f}, \\ \tilde{f} &= \frac{1}{16} (1/\varepsilon - \varepsilon)(\alpha^2 - 1/\alpha^2), \quad \alpha_{\mathbf{k}} = \sqrt{\varepsilon_{\mathbf{k}}/\varepsilon'_{\mathbf{k}}}, \end{aligned} \quad (5.36)$$

where one switches at $t = 0$ the oscillator frequency from ω' to ω and where $\varepsilon'_{\mathbf{k}}$ is the dispersion relation before that quench. The dephasing properties are dominated by the vicinity of $\mathbf{k} = 0$; compare to Fig. 5.3b.

5. Dephasing, the steady state, and its entanglement entropy for integrable systems

ω'	ω	ℓ	m	χ	$d = 1$	$d = 2$	$d = 3$
finite	finite	2	0	$\frac{2-d}{2}$	$\mathcal{O}(\frac{1}{\sqrt{t}})$	$\mathcal{O}(\frac{1}{t})$	$\mathcal{O}(\frac{1}{t})$
0	finite	2	1	$\frac{3-d}{2}$	no	$\mathcal{O}(\frac{1}{\sqrt{t}})$	$\mathcal{O}(\frac{1}{t})$
finite	0	1	2	$\frac{3-d}{1}$	no	no	$\mathcal{O}(\frac{1}{t})$

Table 5.1.: Dephasing properties of the d -dimensional harmonic lattice model (5.34). The system is prepared in the ground state for the oscillator frequency ω' . At $t = 0$, the frequency is switched to ω (*quench* $\omega' \mapsto \omega$). The rightmost columns specify for each kind of quench the resulting decay of the nondiagonal contributions to the subsystem Green's function G_t . The colors in the leftmost columns were chosen as to match those of the corresponding curves for $\tilde{f}$ in Fig. 5.3b. The colors in the rightmost columns match those of corresponding curves in Fig. 5.4.

- If one switches between two noncritical (i.e. finite) values $\omega', \omega > 0$ ($\omega' \neq \omega$), the phase function, which is here just $2\varepsilon_{\mathbf{k}}$, is quadratic around $\mathbf{k} = \mathbf{0}$ corresponding to $\ell = 2$ in (5.29). Also, $1/\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}} = \mathcal{O}(1)$ and $\alpha_{\mathbf{k}}^2 - 1/\alpha_{\mathbf{k}}^2 = \mathcal{O}(1)$ around $\mathbf{k} = \mathbf{0}$, meaning that the amplitude f has no divergence. The characteristic of the point $\mathbf{k} = \mathbf{0}$ in terms of (5.29) is thus $(\ell, m) = (2, 0)$, i.e. $\chi = \frac{2-d}{2}$ and, hence, dephasing is effective with nondiagonal contributions to the subsystem Green's function decaying as $\mathcal{O}(1/\sqrt{t})$ for $d = 1$ and as $\mathcal{O}(1/t)$ for $d > 1$.
- For $\omega' = 0$ and $\omega > 0$, one has $1/\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}} = \mathcal{O}(1)$ but $\alpha_{\mathbf{k}}^2 - 1/\alpha_{\mathbf{k}}^2 = \mathcal{O}(1/k)$ around $\mathbf{k} = \mathbf{0}$, as $\varepsilon_{\mathbf{k}} = \mathcal{O}(k)$. The characteristic in terms of (5.29) is thus $(\ell, m) = (2, 1)$ and consequently one has no dephasing for $d = 1$, dephasing of $\mathcal{O}(1/\sqrt{t})$ for $d = 2$, and of $\mathcal{O}(1/t)$ for $d = 3$.
- For $\omega' > 0$ and $\omega = 0$, one has around $\mathbf{k} = \mathbf{0}$ a linear dispersion $\varepsilon_{\mathbf{k}} = \mathcal{O}(k)$ and hence $1/\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}} = \mathcal{O}(1/k)$, $\alpha_{\mathbf{k}}^2 - 1/\alpha_{\mathbf{k}}^2 = \mathcal{O}(1/k)$, and thus $(\ell, m) = (1, 2)$. So, there is no dephasing for $d = 1$ and 2, and dephasing of $\mathcal{O}(1/t)$ for $d = 3$.

On the Brillouin zone surface there are further isolated zeros of the phase function φ (here just $2\varepsilon_{\mathbf{k}}$) with $\ell = 2$; for $d = 1$ at $k = \pm\pi$, for $d = 2$ at $(\pm\pi, 0)$ and $(0, \pm\pi)$. Due to this and the fact that the amplitude $f_{\mathbf{k}}$ is for all discussed quenches finite at those points ($m = 0$, i.e. $\chi = (m + \ell - d)/\ell = 1 - d/2$), they do not change the dephasing characteristics which we obtained by considering the critical point at $\mathbf{k} = \mathbf{0}$.

Those results were confirmed numerically for $d = 1, 2$ and are summarized in Table 5.1 and Fig. 5.4.

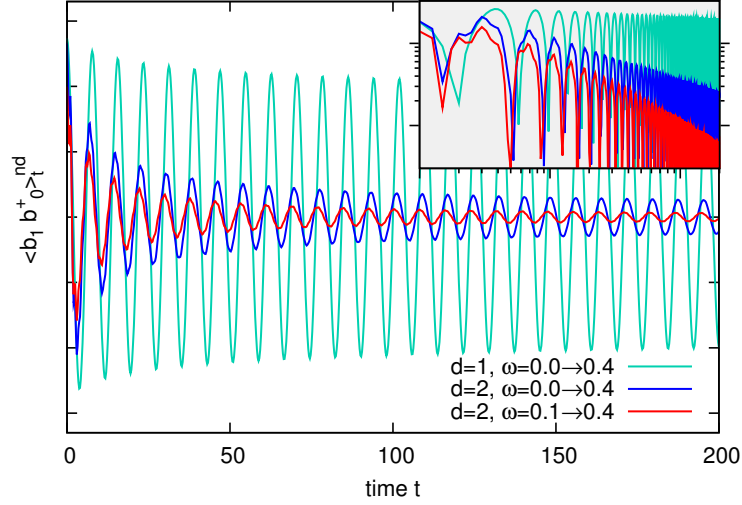


Figure 5.4.: Dephasing in the d -dimensional harmonic lattice model (5.34). As discussed in the text and summarized in Table 5.1, the displayed nondiagonal contributions to the correlator $\langle b_1 b_0^\dagger \rangle_t$ do *not* decay for $d = 1$ and the quench $\omega = 0 \rightarrow 0.4$, decay as $\mathcal{O}(1/\sqrt{t})$ for the same quench in $d = 2$ dimensions, and as $\mathcal{O}(1/t)$ for the quench $\omega = 0.1 \rightarrow 0.4$ in $d = 2$ dimensions. This is confirmed in the double logarithmic plot of the insets.

5.2.5. Hardcore bosons in a one-dimensional box

As a last example, consider free hard-core bosons in a one-dimensional box; the Hamiltonian contains only the hopping term. The system is prepared in the ground state for a box of size $\tilde{L}$ which is switched to $L > \tilde{L}$ at $t = 0$, [191]. The Jordan-Wigner transformation yields a model of free fermions. The transformation between one-particle eigenstates before and after the quench ($|q\rangle$ and $|k\rangle$) is

$$V_{kq} = \langle k|q\rangle = \frac{e^{i(k-q)/2} \sin(\tilde{L}(k-q)/2)}{\sqrt{L\tilde{L}} \sin((k-q)/2)} =: V_{k-q}. \quad (5.37)$$

The weight of $V_{\Delta k}$ is concentrated in the interval $|\Delta k| \lesssim 2\pi/\tilde{L}$. With the Fermi momentum q_F , the initial Green's function $[\mathcal{G}_0^\eta]_{qq'} = \delta_{qq'}(1 - \theta(q_F - |q|))$ is diagonal in the $|q\rangle$ basis and $[\mathcal{G}_0^\eta]_{kk'} = [V\mathcal{G}_0^\eta V^\dagger]_{kk'}$, which appears in (5.16), is hence also concentrated in $|k - k'| \lesssim 1/\tilde{L}$. Thus $|\varphi_{\Delta k}(k)|$ and $|g|$ are very small on the support of $[\mathcal{G}_0^\eta]_{kk'}$, namely $\lesssim 1/\tilde{L}$, such that dephasing is ineffective. In [191], the bosonic momentum distribution $\langle \hat{n}_k \rangle$ was found to relax to the one of the corresponding steady state ensemble $\hat{\varrho}_d$. However, as the dephasing is ineffective, relaxation (5.10) of subsystem density matrices does not occur. This is also visible in the observables: As derived in [195], correlators do not relax to the value predicted by $\hat{\varrho}_d$; see also non-decaying oscillations of $\langle \hat{n}_x \rangle$ in Ref. 41 of [191] and Fig. 10 of [192]. That a particular observable, here $\langle \hat{n}_k \rangle$, may relax anyway is a

different issue. In [195] it was shown for a slightly modified setup how relaxation of $\langle \hat{n}_k \rangle$ occurs.

5.3. Discussion

The dephasing theorem (5.10) confirms the conjectured (5.2), clarifies its interpretation, and devises conditions for its applicability: It is of course not possible that the system converges from an initially pure state to an ensemble (5.2), which is a mixed state of the full system $\Omega \cup \Omega^\perp$. It is rather such that, under the preconditions as given in Sec. 5.1.3, *subsystem states* of Ω converge due to the dephasing effect to *reduced density matrices* of the ensemble (5.2).

Dephasing properties are determined in particular by points where the gradient $\mathbf{g} = \partial_{\mathbf{k}}\varphi$ of the phase function, Eq. (5.18), vanishes or the amplitude f , Eq. (5.16), diverges. Also note that the notion of integrals of motion standing in involution as used for classical systems does not carry over to quantum mechanics, [198]. Hence it was per se not clear what operators $\hat{I}_k$ were to be chosen in the maximum entropy ensemble (5.2). The theorem settles this question.

5.4. Entanglement entropy of the steady state and simulatability

As α_k , Eq. (5.11), becomes finite for finite k regions, the subsystem (entanglement) entropies will finally be dominated by the extensive contribution

$$S_\Omega = \text{Vol } \Omega \sum_k \log[(1 + \zeta e^{-\alpha_k})^{-\zeta}] + o(\text{Vol } \Omega) \quad (5.38)$$

(cmp. also to [112] for the one-dimensional case). As discussed in detail in Sec. 1.5, this means that the required computational resources to simulate such systems on classical computers (via tensor contraction ansatz states as MPS, PEPS, or MERA) scale exponentially in the system size, preventing access to arbitrarily long times. On the other hand, this shows that quenches are a simple tool for the controlled generation of strong (extensive) entanglement.

5.5. Bethe Ansatz integrable systems

In Bethe Ansatz solvable models [20], the transfer matrix $\hat{\tau}(\lambda)$ is conserved for any value of the spectral parameter λ .

$$[\hat{\tau}(\lambda), \hat{\tau}(\lambda')] = 0 \quad \text{and} \quad [\hat{\tau}(\lambda), \hat{H}] = 0 \quad \forall \lambda, \lambda'. \quad (5.39)$$

Initial states $\hat{\varrho}_0$ can be expanded in a $\hat{\tau}(\lambda)$ -eigenbasis $|\lambda\rangle$ and, via time evolution, non-diagonal contributions will attain quickly oscillating phases

$$\hat{\varrho}_t = \sum_{\lambda, \lambda'} e^{(E_\lambda - E_{\lambda'})t/i\hbar} |\lambda\rangle \langle \lambda| \hat{\varrho}_0 |\lambda'\rangle \langle \lambda'|. \quad (5.40)$$

It will be shown elsewhere that, as in the free case, the nondiagonal contributions to the density matrix $\text{Tr}_{\Omega^\perp} \hat{\rho}_t$ of a finite subsystem Ω will under appropriate preconditions decay. Then, the steady state in the thermodynamic limit will, in generalization of (5.10), be given by

$$\lim_{t \rightarrow \infty} \text{Tr}_{\Omega^\perp} \hat{\rho}_t = \text{Tr}_{\Omega^\perp} \hat{\rho}_d, \quad \hat{\rho}_d = \frac{1}{Z} e^{-\int d\lambda \rho(\lambda) \alpha_\lambda \hat{\tau}(\lambda)}, \quad (5.41)$$

where ρ denotes the density of quasiparticles.

5.6. Nonintegrable systems

Whether or how thermalization occurs in nonintegrable systems is in general unclear. Intuitively, information about the initial state gets smeared out by scattering events which are, contrary to the integrable case [199], able to change the quantum numbers of the involved particles and not factorisable. The results above are expected to carry over to nonintegrable cases, if system and initial state allow for a description by an integrable theory of quasiparticles (e.g., Fermi gases and Luttinger liquids) and quasiparticle lifetimes exceed time scales necessary to observe dephasing. In such cases, first relaxation to the steady state of the integrable theory will occur, followed by decay to the thermal ensemble. Numerical results in [200] may be interpreted in this vein.

After finishing this part of the thesis, further investigations for time-evolution after quenches addressed for example the non-integrable Hubbard model in higher dimensions with a dynamical mean field theory approach [201], an interacting model of spinless fermions [202], or the Bose-Hubbard model [203].

Part II.

Simulation of many-particle systems via tensor contraction states

6. Spectral functions in one-dimensional quantum systems at finite temperatures

An application of time-dependent density-matrix renormalization-group simulations (t-DMRG) at finite temperatures is presented. It is demonstrated how a combination of finite-temperature t-DMRG and time-series prediction allows for an easy and very accurate calculation of spectral functions in one-dimensional quantum systems, irrespective of their statistics, for arbitrary temperatures. This is illustrated with spin structure factors of XX and XXX spin- $\frac{1}{2}$ chains. For the XX model we can compare against an exact solution and for the XXX model (Heisenberg antiferromagnet) against a Bethe Ansatz solution and quantum Monte Carlo data.

Strongly correlated quantum systems pose central challenges in theoretical condensed-matter physics. In the case of one-dimensional systems, one now has a full range of techniques to address static and dynamic ground-state properties. However, condensed-matter experiments typically work at finite temperatures that cannot be simply approximated by the ground-state physics, and the low-temperature physics of such systems is of high interest of its own. Due to the homogeneity of the systems under study in space and time, the experimental responses are best represented in momentum-frequency space, as, for example, by spin structure factors

$$S^{\mu\nu}(k, \omega) = \sum_{\ell} e^{ik\ell} \int dt e^{i\omega t} \langle \hat{S}_{\ell}^{\mu}(t) \hat{S}_0^{\nu}(0) \rangle, \quad (6.1)$$

where the average is taken with respect to some finite- T density operator and $[\hat{S}_{\ell}^{\mu}, \hat{S}_{\ell'}^{\nu}] = i\delta_{\ell\ell'}\epsilon_{\mu\nu\gamma}\hat{S}_{\ell}^{\gamma}$. Functions of this form will be referred to as spectral functions in the following; the proposed method does not depend on the specifics. Theoretical approaches to calculate such spectral functions with high accuracy are very limited. On the other hand, experimental progress makes such calculations very timely: For example, due to small neutron flux, neutron-scattering techniques were in the past essentially limited to finding scattering maxima. Now, they have advanced to a degree that both the amplitude and the lineshape, which contain important information on the many-body physics involved, can be investigated with high accuracy (e.g., Refs. [204] and [205]).

For finite-temperature quantum Monte Carlo (QMC) calculations (e.g., positive-definite path integral [49, 62] or stochastic series expansion [50] representation), spectral functions have to be extracted by analytic continuation from imaginary-time results [206], which is ill-conditioned and numerically challenging. In the context of DMRG [66, 124, 68], early

approaches for finite-temperature spectral functions have built on transfer-matrix DMRG [207, 208], which gives thermodynamics for homogeneous infinite systems at high precision. In a first step, analytic continuation techniques as in QMC were employed [209]. In a second development, transfer matrices were evolved in real-time to access autocorrelation functions [210, 211]; the time scales reachable limit resolution in frequency space. While this approach would also be amenable to the prediction techniques used in the following to circumvent this issue, the determination of momentum-space correlators will be particularly easy with the t -DMRG methods [74–76] used here. In an unrelated development, a ground-state DMRG-like technique has been proposed that invokes a random-sampling and averaging procedure [212]. Its feasibility for dynamical quantities has only been tested for very small systems; it is also limited to low temperatures.

In this chapter, a (to my knowledge first) application of t -DMRG at finite temperatures is presented. This technique is limited to finite maximum times t , as entanglement entropy builds up roughly linearly in time, cf. Secs. 1.4 and 1.5. It is shown how to circumvent this limitation by combining t -DMRG with the linear prediction method [213, 214], allowing us to obtain very accurate results for spectral functions with frequency and momentum dependence in the entire temperature range. While the demonstration focuses on a few particular cases, it will be obvious that the approach generalizes straightforwardly.

6.1. Method

6.1.1. DMRG at finite temperature

In recent years, DMRG [66, 124] has emerged as a key method for the ground-state physics of strongly correlated one-dimensional quantum systems [68]. The time-evolution of pure states in one-dimensional strongly correlated spin, bosonic or fermionic models can now be simulated by t -DMRG [74–76] over times 10-100 times longer than the typical inverse energy scale of the problem (e.g., inverse hopping energy). It was quickly demonstrated [77] that this method can be easily extended to the simulation of the static and dynamic behaviors at $T > 0$ by using the purification [215, 216, 67] of the density operator: Any density operator $\hat{\rho}$ of some physical system $\mathcal{H}$ can be encoded by a pure state of a combined physical and ancillary system, $|\rho\rangle \in \mathcal{H} \otimes \mathcal{A}$, such that the density matrix is retained by tracing out $\mathcal{A}$,

$$\hat{\rho} = \text{tr}_{\mathcal{A}} |\rho\rangle\langle\rho|. \quad (6.2)$$

The ancillary system $\mathcal{A}$ can be taken as a copy of the physical state space $\mathcal{H}$; Fig. 6.1. In the case of interest, (unnormalized) thermal density operators $\hat{\rho}_{\beta} = e^{-\beta\hat{H}}$, the corresponding purification can be constructed by an imaginary-time evolution starting from the purification of the (trivial) infinite- T ($\beta = 0$) density operator $\hat{\rho}_0 = \mathbb{1}$. A possible purification for this $\beta = 0$ ensemble is

$$|\rho_0\rangle = \otimes_{\ell=1}^L |\rho_{0,\ell}\rangle \quad \text{with} \quad |\rho_{0,\ell}\rangle = \sum_{\sigma_{\ell}} |\sigma_{\ell}\rangle \otimes |\sigma_{\ell}\rangle', \quad (6.3)$$

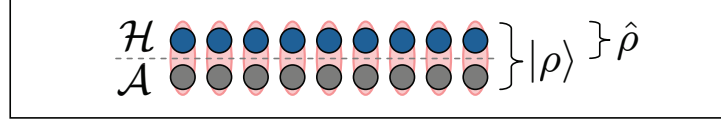


Figure 6.1.: The purification of a density operator $\hat{\rho}$ on a Hilbert space $\mathcal{H}$ is a pure state $|\rho\rangle$ on an enlarged Hilbert space $\mathcal{H} \otimes \mathcal{A}$ such that $\hat{\rho} = \text{tr}_{\mathcal{A}} |\rho\rangle\langle\rho|$. The infinite temperature state $\hat{\rho}_0 \propto \mathbb{1}$ is obtained by preparing each pair of a physical site and the corresponding auxiliary site in a maximally entangled state.

where $\{|\sigma_\ell\rangle\}$ and $\{|\sigma'_\ell\rangle\}$ denote the bases of the physical state space of site ℓ and its associated ancillary state space, respectively. With this, one has $\hat{\rho}_0 = \text{Tr}_{\mathcal{A}} |\rho_0\rangle\langle\rho_0|$. Finite temperatures $\beta > 0$ are reached by imaginary-time evolution

$$\hat{\rho}_\beta = e^{-\beta\hat{H}} = \text{Tr}_{\mathcal{A}} |\rho_\beta\rangle\langle\rho_\beta| \quad \text{with} \quad |\rho_\beta\rangle = e^{-\beta\hat{H}/2} |\rho_0\rangle.$$

Proper normalization is restored by imposing $\langle\rho_\beta|\rho_\beta\rangle = 1$. The mixed state $\hat{\rho}_\beta$ can then be evolved in time as $|\rho_\beta(t)\rangle = e^{-i\hat{H}t} |\rho_\beta(0)\rangle$ and $\hat{\rho}_\beta(t) = \text{Tr}_{\mathcal{A}} |\rho_\beta(t)\rangle\langle\rho_\beta(t)|$.

As a product state, the initial $\beta = 0$ purification $|\rho_0\rangle$ is uncorrelated, and hence, for the DMRG simulation, can be expressed exactly with block Hilbert spaces of dimension $m = 1$. Imaginary-time evolution will introduce correlations, requiring one to increase m . For the evaluation of expectation values, both physical and ancillary degrees of freedom are traced over. As an example, take

$$\begin{aligned} \text{Tr}_{\mathcal{H}}(S_i^z(t)S_j^z(0)\hat{\rho}_\beta) &= \text{Tr}_{\mathcal{H}\otimes\mathcal{A}}(S_i^z(t)S_j^z(0)|\rho_\beta\rangle\langle\rho_\beta|) \\ &= \langle\rho_\beta|e^{i\hat{H}t}S_i^ze^{-i\hat{H}t}S_j^z|\rho_\beta\rangle. \end{aligned} \quad (6.4)$$

While this approach has been found to yield thermodynamic quantities [78] and static correlators [69] at $T > 0$ to very high accuracy, real-time simulations are plagued by the same limitations as at $T = 0$: the propagation of excitations through the system leads to entanglement growth in the purified state. As entanglement entropy is related roughly exponentially to DMRG resources, this strongly limits achievable simulation times (cf. Sec. 1.5), or inversely the ω -resolution for spectral functions, as those are derived by Fourier transformation from the real-time data. In order to circumvent this limitation at very low numerical cost, a linear prediction technique [213, 214] is adapted that has already been employed successfully at $T = 0$ in Ref. [217, 72].

6.1.2. Linear prediction

For a time series of complex data $x_0, x_1, \dots, x_N$ at equidistant points in time $t_n = n \cdot \Delta t$ (and $t_{\text{obs}} := N\Delta t$) one makes a prediction of $x_{N+1}, x_{N+2}, \dots$. In our case, t_{obs} is the (physical) time where the t -DMRG calculation was stopped – usually because the computational cost to simulate further with a given accuracy has become too high. For the

data points beyond $t = t_{\text{obs}}$, linear prediction makes the ansatz

$$\tilde{x}_n = - \sum_{i=1}^p a_i x_{n-i}. \quad (6.5)$$

The (predicted) value $\tilde{x}_n$ at time step n is assumed to be a linear combination of p previous values $\{x_{n-1}, \dots, x_{n-p}\}$. Once the coefficients a_i are determined from the known data, the ansatz is used to calculate (an approximation of) all x_n with $n > N$.

The coefficients a_i are determined by minimizing the least-square error in the predictions over a subinterval $(t_{\text{obs}} - t_{\text{fit}}, t_{\text{obs}}]$ of the known data, i.e. we need to minimize

$$E \equiv \sum_{n \in \mathcal{N}_{\text{fit}}} |\tilde{x}_n - x_n|^2 / w_n \quad (6.6)$$

where $\mathcal{N}_{\text{fit}}$ is the fitting interval $\mathcal{N}_{\text{fit}} = \{n | t_n \in (t_{\text{obs}} - t_{\text{fit}}, t_{\text{obs}}]\}$, and w_n is some weighting function. Here, for the simulations, $w_n \equiv 1$ was chosen. It was found that $t_{\text{fit}} = t_{\text{obs}}/2$ is a robust choice. It is a compromise between choosing t_{fit} small enough to eliminate spurious short-time behavior from the true long-time behavior and choosing t_{fit} large to have a good statistics for the fit and allow for a large number p of coefficients a_i in the ansatz (6.5). Minimization of the error E , Eq. (6.6), with respect to the coefficients a_i yields the system of linear equations

$$R\mathbf{a} = -\mathbf{r}, \quad (6.7)$$

where R and $\mathbf{r}$ are the autocorrelations

$$R_{ji} = \sum_{n \in \mathcal{N}_{\text{fit}}} x_{n-j}^* x_{n-i} / w_n, \quad r_j = \sum_{n \in \mathcal{N}_{\text{fit}}} x_{n-j}^* x_n / w_n.$$

Equation (6.7) is solved by $\mathbf{a} = -R^{-1}\mathbf{r}$. For positive w_n , R is a positive-definite matrix.

One may wonder why the extrapolation to infinite time is possible in this fashion. As demonstrated below, linear prediction generates a superposition of oscillating and exponentially decaying (or growing) terms, a type of time dependence that emerges naturally in many-body physics: Green's functions of the typical form $G(k, \omega) = (\omega - \epsilon_k - \Sigma(k, \omega))^{-1}$ are in time-momentum representation dominated by the poles; e.g., for a single simple pole at $\omega = \omega_1 - i\eta_1$ with residue c_1 , it will read $G(k, t) = c_1 e^{-i\omega_1 t - \eta_1 t}$, and similarly it will be a superposition of such terms for more complicated pole structures. So the ansatz of the linear prediction is well suited for the typical properties of the response quantities we are interested in. Note, however, that the method is not generally applicable for genuine nonequilibrium situations, as, e.g., for the evolution of a local observable after a noninfinitesimal quench of system parameters (cf. Chap. 5). In such cases, typically, too many different frequencies can contribute to the signal, making the ansatz inappropriate.

To see the special form of time-series generated by the prediction, let us introduce vectors $\mathbf{x}_n := [x_{n-1}, \dots, x_{n-p}]^T$ such that (6.5) takes the form

$$\tilde{\mathbf{x}}_{n+1} = A \cdot \mathbf{x}_n, \quad (6.8)$$

with

$$A \equiv \begin{bmatrix} -a_1 & -a_2 & -a_3 & \cdots & -a_p \\ 1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & 1 & 0 \end{bmatrix}. \quad (6.9)$$

Prediction therefore corresponds to applying powers of A to the initial vector $\mathbf{x}_N$. A (right) eigenvector decomposition of A with eigenvalues α_i leads to

$$\tilde{x}_{N+m} = [A^m \cdot \mathbf{x}_N]_1 = \sum_{i=1}^p c_i \alpha_i^m, \quad (6.10)$$

where coefficients c_i are determined from $\mathbf{x}_N$ and the eigenvectors of A . The eigenvalues α_i encode the physical resonance frequencies and dampings. The connection is given as $\alpha_i = e^{i\omega_i \Delta t - \eta_i \Delta t}$. Excluding exponentially growing terms as unphysical, all α_i should obey $|\alpha_i| \leq 1$. In numerical practice, eigenvalues $|\alpha_i| > 1$ may occur, and various remedies exist, all based on the assumption that the corresponding c_i are small. Common manipulations of occurring $|\alpha_i| > 1$ are $\alpha_i \rightarrow \alpha_i/|\alpha_i|$, $\alpha_i \rightarrow 1/\alpha_i^*$, and $\alpha_i \rightarrow 0$. After testing all three, the last option was chosen. When linear prediction is applicable, the choice should not matter (see discussion at the end of Sec. 6.2.1).

From the study of several examples, it was found that the error of the linear prediction is roughly a function of $p \cdot \Delta t$, i.e. p should be adapted to the choice of the time step Δt in the DMRG time evolution. In the simulations, $p \cdot \Delta t = t_{\text{fit}}/2$ was chosen as a compromise between a large p to allow for a superposition of as many different oscillations as possible and a small p to have good statistics for the fit of the coefficients a_i .

At $T = 0$, critical one-dimensional systems exhibit power-law decays in their time-dependent correlators. The superposition of exponential decays is then taken to mimic these power-laws [217]. At finite temperatures, time-dependent correlators $S(k, t)$ decay typically exponentially for large times (due to thermal broadening), making linear prediction especially well-suited for this situation.

6.2. Applications

6.2.1. XX model

The Hamiltonian of the XX model reads

$$\hat{H}_{\text{XX}} = \sum_i (\hat{S}_i^x \hat{S}_{i+1}^x + \hat{S}_i^y \hat{S}_{i+1}^y) + h \sum_i \hat{S}_i^z, \quad (6.11)$$

where the critical field $h = -1$ was chosen. Let us consider the observable

$$S(\ell, t) = \frac{1}{2\pi} \langle [\hat{S}_\ell^-(t), \hat{S}_0^+(0)] \rangle_\beta, \quad (6.12)$$

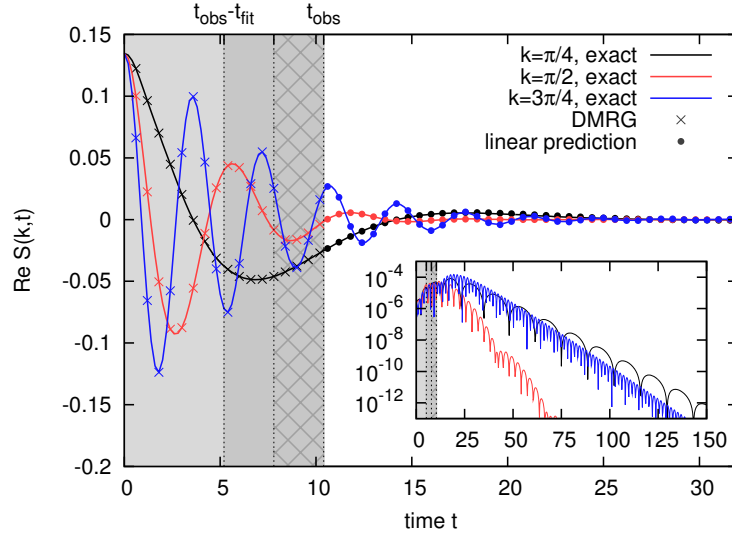


Figure 6.2.: XX model at $\beta = 10$: The exact $\text{Re } S(k, t)$ and the result of DMRG simulation followed by linear prediction are in excellent coincidence. The inset shows the long-time behavior of the deviation to the exact result. At $t = t_{\text{obs}}$, the DMRG simulation was stopped (gray area). For the prediction, the deviation (6.6) of predicted to simulated values was minimized on the interval $(t_{\text{obs}} - t_{\text{fit}}, t_{\text{obs}}]$ (dark gray) with respect to the coefficients a_i in (6.5). The hatched interval $(t_{\text{obs}} - p \cdot \Delta t, t_{\text{obs}}]$, determines the value of the first predicted value at $t = t_{\text{obs}} + \Delta t$.

which is the spectral function of the corresponding model of hardcore bosons. This allows for a detailed analysis of the method, as correlators for this model can be calculated numerically exactly by the evaluation of Pfaffian determinants [218, 219, 69].

The DMRG simulation employed a fourth-order Trotter-Suzuki decomposition and a time step $\Delta t = 0.2$. Deviations $||\rho_{\Delta t}^{\text{exact}} - \rho_{\Delta t}^{\text{DMRG}}||/\Delta t$ between exactly time-evolved state and its DMRG approximation were bounded from above by 0.005 per time unit. A lattice of $L = 100$ sites was used¹. To demonstrate the potential of the prediction method, the calculations were stopped at times $t_{\text{obs}} = 10.4$ for $\beta = 10$ and $t_{\text{obs}} = 26.6$ for $\beta = 50$ (which can be reached with very moderate computational resources corresponding to DMRG block Hilbert spaces of dimension $m \lesssim 200$). For the linear prediction (6.5), the parameter p was chosen as $p = 14$ for $\beta = 10$ and $p = 34$ for $\beta = 50$. The fitting interval was taken from half the maximal computation time onward ($t_{\text{fit}} = t_{\text{obs}}/2$ and $p \cdot \Delta t = t_{\text{obs}}/4$).

In Fig. 6.2 it can be seen that very accurate predictions are possible far into the future. As

¹ The finite temperature causes a finite correlation length in the $t = 0$ state. During time evolution, correlations are built up further only inside causal cones. Hence for small enough β and t , finite-size effects are negligible if measurements are restricted to the middle of the system.

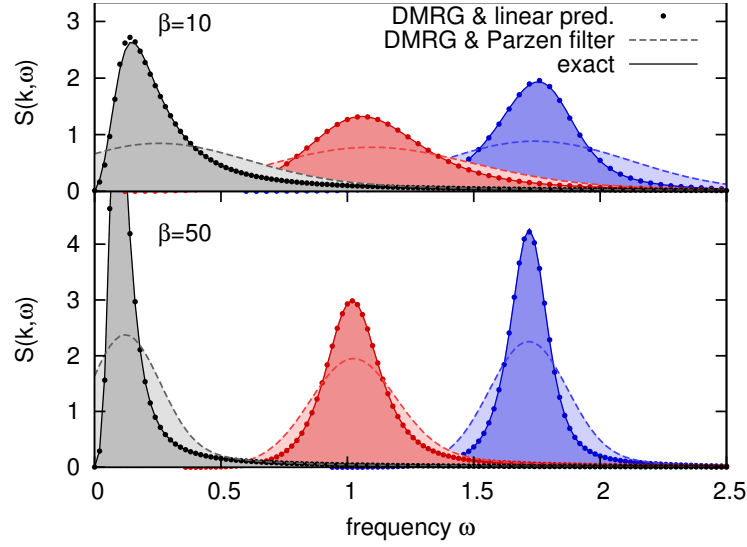


Figure 6.3.: Lineshapes for the XX model at various values of the quasimomentum k (from left to right: $k = \pi/8, \pi/3$, and $3\pi/4$) at $\beta = 10$ and $\beta = 50$: exact (solid lines) and predicted (dots) lineshapes are in excellent agreement. For comparison, Parzen-filtered lineshapes (dashed lines) obtained from (raw) DMRG data are shown.

Fig. 6.3 shows, for both temperatures, lineshapes can be calculated very accurately upon Fourier transformation of the predicted data, allowing for precise experimental analysis. In contrast, even upon windowing (here done by a Parzen filter), the raw data provide completely wrong line maxima and widths. Almost the whole spectral function is reproduced very exactly. The sole exception occurs for values of k very close to zero and π : here, the group velocity vanishes, $d\omega/dk \rightarrow 0$, leading to a very slow decay of correlators which is not captured perfectly for the chosen temperatures and maximum simulation times t_{obs} .

In Sec. 6.1.2, arguments were given for the parameter choice $t_{\text{fit}} = t_{\text{obs}}/2$ and $p \cdot \Delta t = t_{\text{fit}}/2$ for the prediction method. There is one further parameter involved: For the determination of prediction coefficients a_i in (6.5), the autocorrelation matrix R has to be inverted, (6.7), and requires some regularization. To this purpose, one may either add a small regularization constant before the inversion $R^{-1} \rightarrow (R + \varepsilon \mathbb{1})^{-1}$, or project out the eigenspaces with eigenvalues below ε i.e. $R^{-1} \rightarrow (P_\varepsilon R P_\varepsilon)^{-1}$ (pseudo inverse).

In cases where the linear prediction method is not appropriate, or the t_{obs} achievable with t -DMRG is too small, the results of the prediction are generally sensitive to variation of the parameters t_{fit} , p , and ε . In this respect, the pseudo inverse approach $R^{-1} \rightarrow (P_\varepsilon R P_\varepsilon)^{-1}$ is favorable, as it produces stronger variations in the result for small changes in ε , if the linear prediction is not applicable. If the method is applicable, the regularization parameter ε can be varied over several orders of magnitude without effect, but should of course be chosen as small as possible (10^{-7} – 10^{-6} in the simulations). An efficient procedure to fix

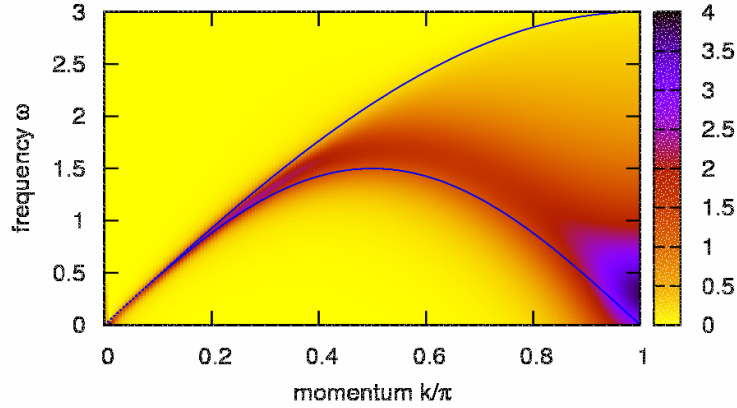


Figure 6.4.: The longitudinal spin structure factor $S^{zz}(k, \omega)$ for the isotropic Heisenberg antiferromagnet at $\beta = 4$ as obtained from DMRG time evolution followed by linear prediction with $t_{\text{obs}} = 7.25$, $t_{\text{fit}} = 3.5$, and $p = 15$. Blue lines mark the bounds (6.15) on the $(T = 0)$ two-spinon spectrum.

ε is to examine plots of the eigenvalues $\alpha_i(k)$ of (6.9) as functions of the quasimomentum k for several ε . For too small ε , noisy scatter and many abrupt jumps appear, resulting in completely wrong lineshapes for some k -values; ε is sufficiently big when $\alpha_i(k)$ shows smooth “band structures” with only a few abrupt jumps. In cases where this is only possible with large ε , the prediction method is not applicable.

6.2.2. Isotropic Heisenberg spin- $\frac{1}{2}$ antiferromagnet

For the Heisenberg antiferromagnet (XXX model)

$$\hat{H}_{\text{HAFM}} = \sum_i \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_{i+1} \quad (6.13)$$

the longitudinal spin structure factor (spectral function)

$$S^{zz}(\ell, t) = \langle \hat{S}_\ell^z(t) \hat{S}_0^z(0) \rangle_\beta \quad (6.14)$$

was calculated. This case is interesting and challenging as already at $T = 0$ a whole continuum of excitations contributes to the spin structure factor as opposed to the simple dispersion of the XX model with a single peak in $S(k, \omega)$ for each momentum. As concluded from $(T = 0)$ Bethe ansatz calculations, the dominant contributions stem from a two-spinon continuum bounded from below and above by [224, 225]

$$\varepsilon_L(k) = \frac{\pi}{2} |\sin k| \quad \text{and} \quad \varepsilon_U(k) = \pi \left| \sin \frac{k}{2} \right|. \quad (6.15)$$

The exact contribution of the two-spinon continuum was derived in Ref. [226, 227] and the contribution of the four-spinon continuum computed in Ref. [220] (see also Ref. [228]).

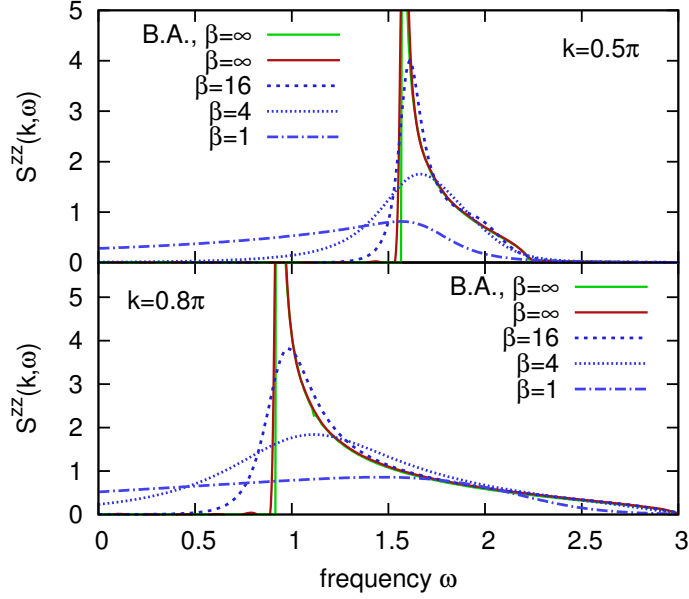


Figure 6.5.: Line shapes of the longitudinal spin structure factor $S^{zz}(k, \omega)$ for the isotropic Heisenberg antiferromagnet as obtained from DMRG and linear prediction at finite T , compared to the $T = 0$ Bethe ansatz result. The Bethe ansatz data (“B.A.”, provided by J.-S. Caux [220]) comprises the two- and four-spinon contributions, accounting for about 98% of the total weight.

The t -DMRG calculation was done for a lattice of 128 sites¹, with a fourth-order Trotter-Suzuki decomposition and time steps $\Delta\beta = \Delta t = 0.125$. The truncation error $\chi^2 = \sum_{i>m} \lambda_i^2$ (χ is the 2-norm of the discarded Schmidt coefficients λ_i) was chosen as $\chi^2 \leq 10^{-12}$ during the cooling and $\chi^2 \leq 10^{-10}$ during the real-time evolution, resulting in a maximum DMRG block Hilbert-space dimension of $m \lesssim 1200$ for the maximum simulation times $t_{\text{obs}} = 6.25, 7.25, 10.5$ at $\beta = 1, 4, 16$, respectively. The parameters for the linear prediction (6.5) were correspondingly chosen as $p = 13, 15, 21$ ($p \cdot \Delta t = t_{\text{obs}}/4$) and $t_{\text{fit}} = t_{\text{obs}}/2$.

The result of DMRG simulation, combined with linear prediction is displayed in Figs. 6.4 and 6.5. The structure factor converges for $\beta \rightarrow \infty$ to the $T = 0$ Bethe ansatz results from Ref. [220].

Fig. 6.6 illustrates robustness of the linear prediction against variation of the corresponding parameters. Changing the regularization parameter by a factor of 10 or the length $p \cdot \Delta t$ of the prediction interval by a factor 1.5 has no visible effect.

There is no Bethe ansatz result available for $T > 0$. Instead, Figs. 6.7 and 6.8 compare to recent quantum Monte Carlo (QMC) data [221]. QMC simulations yield the spin structure factor $S^{\mu\nu}(k, \tau)$ on the imaginary-time axis. This observable can be determined to very

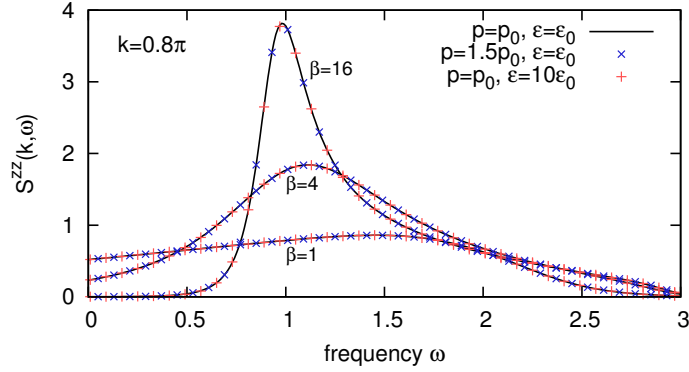


Figure 6.6.: Testing the robustness of the linear prediction method at the example of $S^{zz}(k, \omega)$. The black curves ($p = p_0$ and $\varepsilon = \varepsilon_0$) correspond to the same DMRG data as in Fig. 6.5 ($\Delta\beta = \Delta t = 0.125$; for $\beta = 1, 4, 16$, the prediction parameters were chosen as $p_0 = 13, 15, 21$ and $\varepsilon_0 = 10^{-7}, 10^{-7}, 10^{-6}$, respectively). The blue tilted crosses correspond to simulations where the length $p \cdot \Delta t$ of the prediction interval was increased by a factor of 1.5. The red crosses correspond to calculations where the regularization parameter ε for the inversion of the autocorrelation matrix R was increased by a factor of 10.

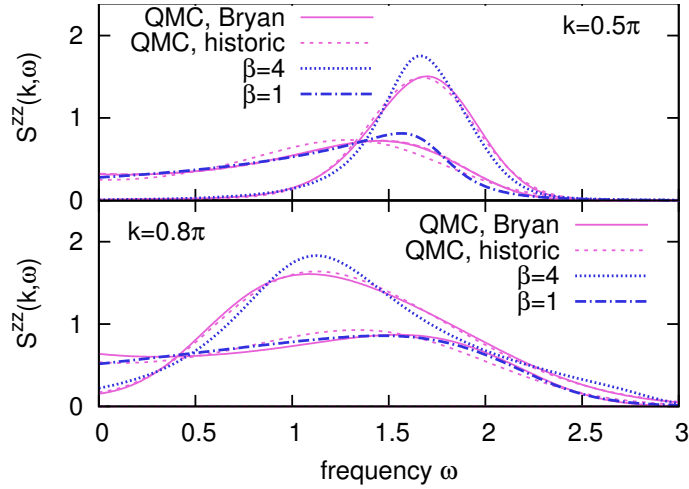


Figure 6.7.: Comparison of the longitudinal spin structure factor $S^{zz}(k, \omega)$ for the isotropic Heisenberg antiferromagnet as obtained from DMRG and linear prediction on the one hand, and QMC and the maximum entropy method on the other hand (provided by S. Grossjohann [221]). The maximum deviation is about 20%. Labels “Bryan” and “historic” refer to the maximum entropy methods of Refs. [222] and Ref. [223], respectively.

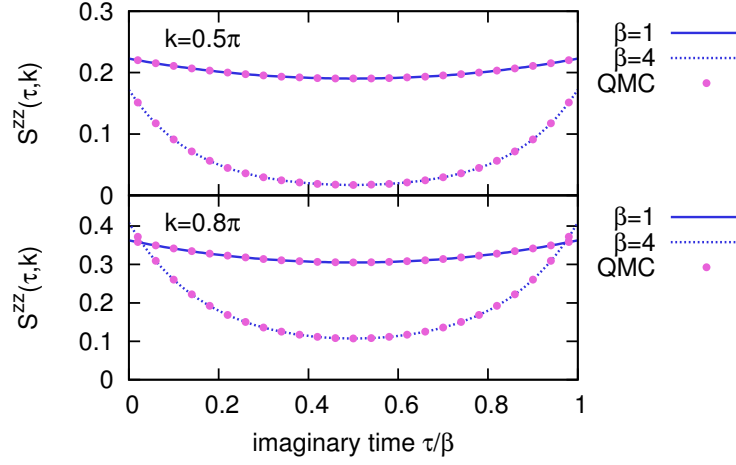


Figure 6.8.: Comparison of the longitudinal spin structure factor $S^{zz}(k, \tau)$ on the imaginary-time axis. DMRG with linear prediction (lines) and QMC [221] (dots) agree very well (maximum discrepancy of $\sim 5 \cdot 10^{-4}$). It is to be concluded that the deviations in $S^{zz}(k, \omega)$ stem from the ill-conditioned analytic continuation which has to be carried out for the QMC data and amplifies small discrepancies.

high precision. The actual quantity of interest is however $S^{\mu\nu}(k, \omega)$, where

$$S^{\mu\nu}(k, \tau) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega e^{-\omega\tau} S^{\mu\nu}(k, \omega). \quad (6.16)$$

To obtain $S^{\mu\nu}(k, \omega)$ from $S^{\mu\nu}(k, \tau)$, one can employ several variants of the maximum entropy method (see, e.g., Ref. [206] for a review). The longitudinal spin structure factor $S^{zz}(k, \omega)$, Fig. 6.7, shows a maximum deviation of about 20%. If one compares however on the imaginary-time axis, $S^{zz}(k, \tau)$ given in Fig. 6.8, QMC and DMRG with linear prediction (the DMRG data was transformed according to (6.16)) agree with a maximum deviation of $\sim 5 \cdot 10^{-4}$. The discrepancy of the corresponding data for $S^{zz}(k, \omega)$, is hence to be attributed to the fact that the maximum entropy method, employed to transform the QMC data to frequency space, is ill-conditioned. This is due to the exponential in (6.16). Small errors of $S^{zz}(k, \tau)$ get blown up by the numerical analytic continuation.

6.3. Discussion

It has been demonstrated how a combination of finite-temperature t -DMRG and linear prediction allows for a very accurate calculation of spectral functions, at finite temperatures. The method is for one-dimensional systems favorable to the usual QMC approach: As t -DMRG has no sign problem, fermionic systems are also directly accessible. Also, no analytic continuation of correlators as in QMC calculations is necessary. As opposed to

6. *Spectral functions in one-dimensional quantum systems at finite temperatures*

some other approaches, the proposed method works over the entire temperature regime. An attractive feature of the method is provided by the increasing availability of t -DMRG codes – which need only minor modification to simulate at finite temperatures – and the simplicity of the numerically inexpensive prediction method.

7. Dynamical reordering for the evaluation of causal circuits of fermionic isometries

A natural way to obtain fermionic variants of tensor product type ansatz states is to replace the tensors by fermionic operators. In this chapter the focus is on fermionic versions of the multiscale entanglement renormalization ansatz which are circuits of fermionic unitaries with a causal cone. This can be employed to simulate strongly correlated fermions in higher dimensions. To work with such states on a classical computer it is necessary to represent the components of the circuit in a appropriate representation – typically the occupation number representation. Doing so in a naïve way for dimensions $d > 1$, due to the transformation, nonlocal Jordan-Wigner string operators appear. A mode reordering scheme is presented that avoids the appearance of any Jordan-Wigner string operators outside the causal cone, providing, hence, a local way of computing local expectation values. Primitives of such a reordering scheme are highlighted. The scheme gives rise to a variational description of fermionic models that, in comparison to quantum Monte Carlo simulations, does not suffer from a sign problem.

Strongly correlated quantum lattice models pose some of the most intriguing problems in quantum physics, presumably being at the basis of phenomena such as high-temperature superconductivity. To theoretically describe such models is often very difficult, an obvious obstacle being the prohibitive dimension of Hilbert space even for moderately sized systems when naively representing ground states. In recent years, it has increasingly become clear, however, that typical ground states of physically meaningful local models are lurking in some corner of Hilbert space, one that can often even be identified. Hence to faithfully describe such a state, even though it may be impossible to parametrize the entire physical space, one merely has to parametrize those quantum states from the relevant set (or good approximations to it), requiring significantly fewer parameters, cf. Chap. 1. The most prominent and to date most powerful incarnation of this idea is provided by the *density-matrix renormalization group* (DMRG) method [66, 68], requiring only linearly many parameters in the system size, but still giving an exceptionally good description of gapped one-dimensional spin chains and a very reasonable one for critical chains.

To realize such an idea in higher-dimensional systems is significantly more difficult, although a lot of progress was made in recent years [119, 118, 120, 125, 229, 128, 230–232, 129] specifically when it comes to generalizing DMRG ideas to higher dimensions (cf. Sec. 1.5), including variations of *tensor product ansätze* or *projected entangled pair*

states (PEPS) [116–119], or circuits of the *multiscale entanglement renormalization ansatz* (MERA). This is a scale invariant approach related real-space renormalization [34], and proposed first in Ref. [120].

To describe higher dimensional fermionic systems, such as the Fermi-Hubbard model itself [233] in such a fashion, appears particularly promising, but also particularly challenging. Here, other key methods of describing quantum lattice models like the powerful quantum Monte-Carlo method are hampered by the sign problem [49, 62, 63]. Surely, fermionic models can readily be represented as spin models, yet at the expense of losing locality (or by doubling the degrees of freedom and increasing the locality region of Hamiltonians [234]). If one considers a term $\hat{f}_j^\dagger \hat{f}_k$, $j < k$, then its spin representation under the *Jordan-Wigner transformation* (JWT) is

$$\sigma_j^- \otimes \bigotimes_{j < l < k} \sigma_l^z \otimes \sigma_k^+.$$

For a pair of nearest neighbor sites $\langle j, k \rangle$ on an $L \times L$ lattice, the occurring *string* operator that is supported not only on the spins associated with j and k , but in fact all spins between j and k , will typically have a length of order L . It should be clear that for a two-dimensional model no order can be chosen to let this apparent problem disappear.

This chapter presents a method to study strongly correlated fermionic models using a fermionic variant of MERA, i.e., circuits of fermionic unitary gates with causal cones of bounded size, in a way that is not overburdened by string operators at all.

When describing the system and computing local expectation values, one has to deal with operators having an identical support as compared to that of a corresponding spin system (fermionic gates of the circuit replaced by regular ones), and strings can be made to disappear. The *causal cone* is, e.g., during the evaluation of a local observable, formed by those unitaries of the circuit that cannot be canceled with their conjugates due to the presence of the observable; cmp. Fig. 7.1. The key point of the suggested approach is to acknowledge that while any fixed mode ordering will give rise to the above problem, we are not forced to keep the order fixed during the evaluation of the circuit. Instead, one can employ a *dynamical reordering* of the fermionic modes in the essential part of the lattice (e.g., the causal cone in the evaluation of local expectation values), reordering and projecting out particles “on the fly”, in *dynamical Jordan-Wigner transformations*.

7.1. Physical algebra

The following three sections prepare the ground of the dynamical reordering idea. The algebra $\mathcal{G}(\mathcal{L})$ of a set of n fermionic modes is spanned by products of anticommuting fermionic operators $\{\hat{f}_j, \hat{f}_j^\dagger : j = 1, \dots, n\}$, with

$$\{\hat{f}_j, \hat{f}_k\} = 0, \{\hat{f}_j, \hat{f}_k^\dagger\} = \delta_{j,k}. \quad (7.1)$$

Physical operators form the subalgebra $\mathcal{F}(\mathcal{L})$, the so-called *physical algebra*, of operators respecting the fermion number parity [235–237]. Each element commutes with the

fermion number parity operator $(-1)^{\hat{N}}$. In practical terms, this means that they are even polynomials in the fermionic creation and annihilation operators. Hence, the physical algebra splits into a direct sum of an even and an odd part,

$$\mathcal{F}(\mathcal{L}) = \mathcal{F}^{(\text{even})}(\mathcal{L}) \oplus \mathcal{F}^{(\text{odd})}(\mathcal{L}). \quad (7.2)$$

For a subset $\mathcal{I} \subset \mathcal{L}$ of some sites, one the corresponding physical algebra is denoted by $\mathcal{F}(\mathcal{I})$ and contains all $\hat{f}_j, \hat{f}_j^\dagger$ with $j \in \mathcal{I}$.

7.2. Fermionic MERA

A *fermionic unitary* is a parity-preserving unitary gate acting on fermionic modes, $\hat{U} = e^{i\hat{h}}$, where $\hat{h} \in \mathcal{F}(\mathcal{L})$ is a hermitian operator. In the considered circuits, unitaries are *local*, i.e., have a small support $\mathcal{I}$ independent of n (e.g., two sites) such that $\hat{U} \in \mathcal{F}(\mathcal{I})$. A fermionic MERA is now an ordered product of such fermionic unitaries and has a causal structure, i.e. causal cones for which the size of every cross-section is bounded; see below. This chapter focuses on *conjugation* as necessary for the evaluation of expectation values of local observables $\hat{A} \in \mathcal{F}(\mathcal{L})$. So we want to evaluate local observables $\hat{A}$, with respect to fermionic MERA states that have been prepared by applying a fermionic unitary circuit to the vacuum state $|\emptyset\rangle$,

$$E = \langle \emptyset | \dots \hat{U}_2 \hat{U}_1 \hat{A} \hat{U}_1^\dagger \hat{U}_2^\dagger \dots | \emptyset \rangle, \quad (7.3)$$

or by applying it to some other product state with odd fermion number parity, e.g., $\hat{f}_n^\dagger |\emptyset\rangle$ instead of $|\emptyset\rangle$. In the fermionic MERA the top layer defines the parity, similar to fixing the topological degrees of freedom in Kitaev's toric code [238]. In fact, there is a natural discrete time label t in a circuit, in that $t = 0, \dots, T$ labels the time at which a single gate is being applied. The mentioned *causal cone* (see Fig. 7.1), is formed by those unitaries in the circuit that cannot be sequentially canceled with their conjugates from the dual vector in Eq. (7.3) due to the presence of the local observable $\hat{A}$. Efficient schemes will have a causal cone of a fixed width, in that a local operator will only touch for each time step a constant number of unitaries. The sequence of sequentially computing the expectation values respecting the discrete time order gives rise to a *contraction*. One can also allow for time steps where partial projections are applied onto the fermionic vacuum in some mode.

Let us now turn to aspects that are specific for fermions. An important property for the elements of disjoint sub-algebras $\hat{U} \in \mathcal{F}(\mathcal{I})$ and $\hat{V} \in \mathcal{F}(\mathcal{J})$, $\mathcal{I} \cap \mathcal{J} = \emptyset$, is that their elements commute:

$$[\hat{U}, \hat{V}] = 0.$$

This has the important consequence that just as for spin systems, all unitaries outside a causal cone can be canceled, and the fermionic variant inherits the same cone as the spin system. For details on MERA and unitary circuits, see also Refs. [120, 125, 229, 128, 230]. As shown in the following, the computation of the expectation value Eq. (7.3) can be done without having to deal with string operators outside the causal cone.

7.3. Jordan-Wigner transformations

In a numerical implementation, fermionic operators will be encoded in an occupation number representation: This representation necessarily depends on the chosen order of the fermionic modes. As it will be necessary to change the ordering of the fermionic modes at different times, it makes sense to first highlight the status of the JWT. For the entire system $\mathcal{L}$ one can take some order O corresponding to an element of the symmetric group S_n , for example the trivial order $O = (1, \dots, n)$. For this order O , a basis for the Hilbert space is given in the *occupation number representation*,

$$|i_1, \dots, i_n\rangle_O = (\hat{f}_{O_1}^\dagger)^{i_1} \dots (\hat{f}_{O_n}^\dagger)^{i_n} |\emptyset\rangle, \quad (7.4)$$

giving an identification of the total Hilbert space with the $(\mathbb{C}^2)^{\otimes n}$, the Hilbert space of n spins $1/2$. Expressing fermionic operators in the occupation number representation amounts to a map $J_O : \mathcal{G}(\mathcal{L}) \rightarrow M(\mathcal{L})$ where $M(\mathcal{L})$ is the algebra of linear operators on $(\mathbb{C}^2)^{\otimes n}$. This map is the well-known *Jordan-Wigner transformation* (JWT), depending on $\mathcal{L}$ and the chosen order $O \in S_n$ of the corresponding fermionic modes. For example, for an annihilation operator it yields

$$J_O(\hat{f}_{O_k}) = \left(\bigotimes_{l=1}^{k-1} \sigma_l^z \right) \otimes \sigma_k^+, \quad (7.5)$$

where $\sigma_k^{x,y,z}$ denote the familiar Pauli operators and $\sigma_j^+ = (\sigma_j^x + i\sigma_j^y)/2$. In this light, a JWT simply gives fermionic operators in the occupation number (or spin) representation for a given ordering O .

Local fermionic operators are identified with *nonlocal* operators in the respective spin systems. Also, physical operators contain strings that depend on the order chosen. Consider a local *physical* operator acting on sites $\mathcal{I}$, the spin representation will in general also be supported on the spins in between with respect to order O . E.g., for the local fermionic number operator one finds $J_O(\hat{f}_{O_j}^\dagger \hat{f}_{O_j}) = \sigma_j^z$, but the occupation number representation of $\hat{f}_{O_j}^\dagger \hat{f}_{O_k}$

$$J_O(\hat{f}_{O_j}^\dagger \hat{f}_{O_k}) = \sigma_j^- \otimes \bigotimes_{j < l < k} \sigma_l^z \otimes \sigma_k^+ \quad (7.6)$$

with $j < k$ contains a *string* of Pauli operators on $[j, k]$.

For physical operators $\hat{A} \in \mathcal{F}(\mathcal{L})$ conservation of the fermion number parity manifests itself in the occupation number representation for an ordering O as follows: Splitting the basis (7.4) into two parts, depending on the parity of $\sum_k i_k$, the spin representation $A = J_O(\hat{A})$ of an operator $\hat{A}$ attains the form

$$A = A^{(\text{even})} \oplus A^{(\text{odd})}. \quad (7.7)$$

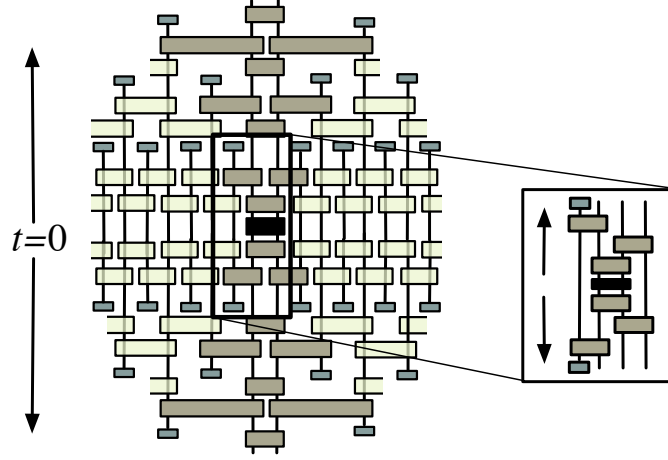


Figure 7.1.: Example for the evaluation of a local observable (central black box) with respect to a fermionic MERA (gray boxes). Each gray box represents a single fermionic unitary. The ones in dark gray compose the causal cone of the observable, all other lie outside of it and cancel each other. Only for conceptual clarity, a 1D MERA is depicted, and not a two-dimensional one, for which dynamical reordering becomes relevant.

7.4. Dynamical reordering

The new scheme to contract a fermionic unitary circuit to be described in the following will be called *dynamical reordering*. It is demonstrated that the contraction can be done with essentially the same complexity compared to the corresponding spin circuit: For the contraction of the unitary circuit, a “time order” is introduced, with $t = 0$ corresponding to the local operator $\hat{A}$ itself. In each step exactly one operation is executed (like adding modes, partially projection, or conjugation with a unitary). The general idea of dynamical reordering is to order only the modes we are currently using (inside the causal cone) at a time t in a non-trivial fashion, with order O^t explicitly dependent on t . As we proceed, new modes appear in the causal cone, and they are added to the description. When they are discarded (e.g., due to projection), they are removed from the description O^t as t evolves. Hence, one arrives at an entirely local description of the fermionic tensor network, without encountering any string operators outside the cone. To do so one can apply the subsequent rules, providing a complete set of primitives, required to contract the unitary circuit. The rules are formulated for the occupation number representations of the participating fermionic operators, as they would be stored for a numerical implementation.

7.4.1. Contraction primitives

(a) *Local representation of fermionic local operators:*

Consider a local operator $\hat{A} \in \mathcal{F}(\mathcal{I})$, that is, it is an even polynomial in the operators

$\{\hat{f}_j, \hat{f}_j^\dagger\}$ for $j \in \mathcal{I}$. The spin representation of the fermionic operator $\hat{A}$ in order O is given by

$$A = J_O(\hat{A}). \quad (7.8)$$

This representation only involves $k = |\mathcal{I}|$ spins.

(b) *Reordering fermionic modes:*

Consider some fermionic operator $\hat{A}$ and an order O^t at some time t . The new spin representation at a time $t + 1$ in the new swapped order O^{t+1} reads,

$$J_{O^{t+1}}(\hat{A}) = p J_{O^t}(\hat{A}) p, \quad (7.9)$$

with $p = \prod_i \mathbb{1} \otimes s_{O_i^t, O_{i+1}^t} \otimes \mathbb{1}$

$$s_{O_i^t, O_{i+1}^t} = |0, 0\rangle\langle 0, 0| + |0, 1\rangle\langle 1, 0| + |1, 0\rangle\langle 0, 1| - |1, 1\rangle\langle 1, 1|, \quad (7.10)$$

where the i are chosen such that the corresponding sequence of nearest-neighbor pair permutations of modes gives rise to the overall permutation $O^{t+1} = \pi(O^t)$; so familiar fermionic swaps can be applied to the local spin representation.

(c) *Prepending fermionic modes:*

Let us have an operator $\hat{A}$ at some time t , represented as $A = J_{O^t}(\hat{A})$ in the order O^t . Prepending a new fermionic mode yields the new order $O^{t+1} = (k, O^t)$. Then the new representation of $A' = J_{O^{t+1}}(\hat{A})$ is given by

$$\begin{aligned} (A')^{(\text{even})} &= |0\rangle\langle 0| \otimes A^{(\text{even})} + |1\rangle\langle 1| \otimes A^{(\text{odd})}, \\ (A')^{(\text{odd})} &= |0\rangle\langle 0| \otimes A^{(\text{odd})} + |1\rangle\langle 1| \otimes A^{(\text{even})}. \end{aligned} \quad (7.11)$$

in the even and odd sectors, i.e. $A' = \mathbb{1} \otimes A$.

(d) *Conjugation with fermionic unitaries having the same support:*

Consider a subset of modes $\mathcal{I}$ at time t . Let $\hat{U}, \hat{A} \in \mathcal{F}(\mathcal{I})$ be fermionic operators with support in $\mathcal{I}$. Then,

$$J_{O^{t+1}}(\hat{U} \hat{A} \hat{U}^\dagger) = J_{O^t}(\hat{U}) J_{O^t}(\hat{A}) J_{O^t}(\hat{U}^\dagger) \quad (7.12)$$

if the same order $O^{t+1} = O^t$ is taken. If $\hat{U}$ is stored in a different order, the permutation rule has to be applied first.

(e) *Partial trace over the first mode:* Let us have some operator $\hat{A}$ at time t in order O^t , and trace out the first mode O_1^t , i.e. $O^t = (O_1^t, O^{t+1})$. Then the spin representation of the resulting fermionic operator is

$$\begin{aligned} J_{O^{t+1}}(\text{Tr}_{O_1^t} \hat{A}) &= \sum \langle i, j_2, \dots, j_k | J_{O^t}(\hat{A}) | i, i_2, \dots, i_k \rangle \\ &\times |j_2, \dots, j_k\rangle \langle i_2, \dots, i_k|, \end{aligned} \quad (7.13)$$

where $k = |O^t|$.

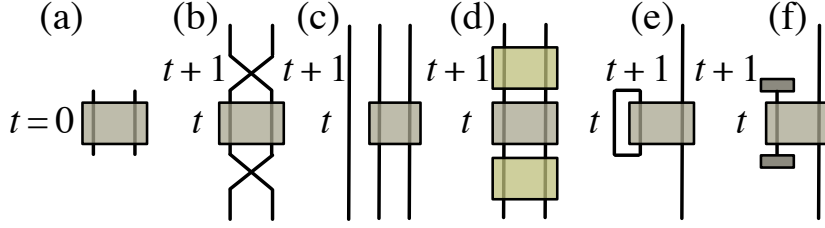


Figure 7.2.: The basic primitives described in the text of (a) expressing local gates in an occupation number representation, (b) reordering fermionic modes, (c) adding fermionic modes, (d) conjugating with fermionic unitaries, (e) partial traces, and (f) partial projections.

(f) *Partial projection over the first mode:*

Let us consider the same orderings O^t and O^{t+1} as for rule (e), but instead of tracing out mode $r = O_1^t$ from operator $\hat{A}$, let us now consider the projection of the mode to the empty state $|0\rangle$ or the state of a filled mode $|1\rangle$. The corresponding projectors in $\mathcal{F}(\mathcal{I})$ are $\hat{P}_r^{(0)} = \hat{f}_r \hat{f}_r^\dagger$ and $\hat{P}_r^{(1)} = \hat{f}_r^\dagger \hat{f}_r$, respectively. Hence the projected fermionic operators are $\hat{P}_r^{(i)} \hat{A} \hat{P}_r^{(i)}$ with $i = 0, 1$. Their occupation number representations follow by applying the partial trace (7.13):

$$J_{O^{t+1}}(\text{Tr}_r \hat{P}_r^{(i)} \hat{A} \hat{P}_r^{(i)}) = \sum |j_2, \dots, j_k\rangle \langle i_2, \dots, i_k| \times \langle i, j_2, \dots, j_k | J_{O^t}(\hat{A}) | i, i_2, \dots, i_k \rangle. \quad (7.14)$$

7.4.2. Proofs for the contraction rules

ad (b) To prove the reordering rule for two modes with labels j, k with $j = O_i^t$ and $k = O_{i+1}^t$, i.e., two modes that are neighboring in the order O^t , one needs to show that

$$J_{O^t}(\hat{S}_{j,k} \hat{A} \hat{S}_{j,k}^\dagger) = s_{j,k} J_{O^t}(\hat{A}) s_{j,k}^\dagger = J_{O^{t+1}}(\hat{A}), \quad (7.15)$$

where $\hat{S}_{j,k}$ acts as $\hat{S}_{j,k} \hat{f}_j \hat{S}_{j,k}^\dagger = \hat{f}_k$ and $\hat{S}_{j,k} \hat{f}_k \hat{S}_{j,k}^\dagger = \hat{f}_j$. One finds

$$\hat{S}_{j,k} = \mathbb{1} - \hat{f}_j^\dagger \hat{f}_j - \hat{f}_k^\dagger \hat{f}_k + \hat{f}_j^\dagger \hat{f}_k + \hat{f}_k^\dagger \hat{f}_j, \quad (7.16)$$

see Ref. [236, 237]. Its spin representation $s_{j,k} = J_{O^{t+1}}(\hat{S}_{j,k})$ is given by

$$s_{j,k} = |0, 0\rangle \langle 0, 0| + |0, 1\rangle \langle 1, 0| + |1, 0\rangle \langle 0, 1| - |1, 1\rangle \langle 1, 1|. \quad (7.17)$$

The reordering rule for more than two modes follows by iteration.

ad (c) To derive the rule for adding modes, note that the local JWT gives

$$J_{O^t}(\hat{f}_{O_k^t}) = (\otimes_{l=1}^{k-1} \sigma_l^z) \otimes \sigma_k^+, \quad (7.18)$$

and hence one obtains for $O^{t+1} = (x, O^t)$ that

$$J_{O^{t+1}}(\hat{f}_{O_{k+1}^{t+1}}) = J_{O^{t+1}}(\hat{f}_{O_k^t}) = \sigma_1^z \otimes J_{O^t}(\hat{f}_{O_k^t}). \quad (7.19)$$

Exploiting the conservation of the fermion number parity for any operator $\hat{A} \in \mathcal{F}(\mathcal{I})$, it follows that

$$J_{O^{t+1}}(\hat{A}) = \sum_{\nu} (\sigma_1^z)^{2\nu} \otimes J_{O^t}(\hat{A}_{\nu}) = \mathbb{1} \otimes J_{O^t}(\hat{A}), \quad (7.20)$$

where $\hat{A}_{\nu}$ collects all monomial terms of degree 2ν such that $\hat{A} = \sum_{\nu} \hat{A}_{\nu}$. With $A' = J_{O^{t+1}}(\hat{A})$ and $A = J_{O^t}(\hat{A})$, for the even and odd sectors, this gives

$$(A')^{(\text{even})} = |0\rangle\langle 0| \otimes A^{(\text{even})} + |1\rangle\langle 1| \otimes A^{(\text{odd})}, \quad (7.21)$$

and similarly $(A')^{(\text{odd})} = |0\rangle\langle 0| \otimes A^{(\text{odd})} + |1\rangle\langle 1| \otimes A^{(\text{even})}$.

ad (e) To show the rule for the fermionic partial trace (7.13), note that for any operator $\hat{B}$ that does not act on mode O_1 , i.e. $\hat{B} \in \mathcal{F}(\mathcal{I} \setminus \{O_1\})$, matrix elements obey

$${}_O \langle i_1, \dots, i_k | \hat{B} | j_1, \dots, j_k \rangle_O = \delta_{i_1, j_1} {}_{O'} \langle i_2, \dots, i_k | \hat{B} | j_2, \dots, j_k \rangle_{O'}, \quad (7.22)$$

where $O = (O_1, O')$ and $k = |O|$. With the definition

$$\text{Tr}_{O_1}(\hat{A}) = {}_O \langle j_1, j_2, \dots, j_k | \hat{A} | j_1, i_2, \dots, i_k \rangle_O \\ |j_2, \dots, j_k \rangle_{O'} {}_{O'} \langle i_2, \dots, i_k |, \quad (7.23)$$

it follows that $\text{Tr}(\hat{A}\hat{B}) = \text{Tr}(\text{Tr}_{O_1}(\hat{A})\hat{B})$ for any $\hat{A} \in \mathcal{F}(\mathcal{I})$. This means that the given expression (7.23) for Tr_{O_1} is the (fermionic) partial trace for mode O_1 . The resulting occupation number representation $J_{O'}(\text{Tr}_{O_1} \hat{A})$ of the partial trace is given in Eq. (7.13).

Rules (c), (e), and (f) were given for the case where only the very first mode O_1 of the ordering is affected (i.e., partial trace of the first mode etc.). Combining those rules with the rule for reordering modes, they are generalized to the case where an arbitrary mode O_j is affected. In the corresponding expressions in the occupation number representation this results in extra sign factors. For the generalization of rule (d), note that when one wants to perform a contraction in which the support is not the same for the two involved operators, one can add the corresponding modes in both operators, reorder and apply rule (d).

7.4.3. Consequences

The main point now is that if one follows this recipe of rules (a-f), and keeps only local descriptions at each time, involving exactly the non-trivial support, one gets an identical value for E in Eq. (7.3) as if one had performed a global Jordan-Wigner transformation and computed it – then with a significant overhead in complexity.

With the basic building blocks, rules (a-f), one can thus contract causal fermionic circuits, as in Fig. 7.1, and also build, e.g., reduced density matrices for MERA [229, 128]. One hence arrives at the following observation:

Observation (Computation of expectation values): *When computing expectation values*

$$E = \langle \Psi | \dots \hat{U}_2 \hat{U}_1 \hat{A} \hat{U}_1^\dagger \hat{U}_2^\dagger \dots | \Psi \rangle \quad (7.24)$$

where the fermionic circuit $\hat{U} = \hat{U}_1 \hat{U}_2 \dots$ prepares a MERA state from an elementary (unentangled) state vector $|\Psi\rangle$, the support of the causal cone in each time step is exactly the same as if one had a spin system with the same topology at each time. Hence, such a fermionic circuit acting on a higher-dimensional fermionic system can be described entirely locally, using the above rules, with the same time and memory complexity.

For some important circuits one also allows for general isometries, which in our case here are treated as unitaries with a subsequent partial projection. As it turns out, general isometries also can be taken account of without this detour, by directly contracting appropriately ordered fermionic operators. One can show that indeed the memory requirements remain unchanged and that the operational overhead is small, and results solely from the necessity of reordering the spin representation of the operators encountered during the contraction. This gives rise to a more general theory of fermionic operator circuits; see Chapter 8.

7.5. Time evolution

One also finds the following: For the time evolution (both real and imaginary) of local fermionic Hamiltonians, one aims at determining updates of each of the fermionic unitaries forming the circuit such that $(\hat{U}'_1)^\dagger (\hat{U}'_2)^\dagger \dots |\Psi\rangle$ is an optimal approximation to the evolved state $e^{x\hat{H}} \hat{U}_1^\dagger \hat{U}_2^\dagger \dots |\Psi\rangle$. This can be done, using the above rules.

7.6. Summary

In this chapter, a time-adaptive Jordan-Wigner transformation (dynamical reordering) technique has been introduced. It helps to contract fermionic unitary circuits, in particular expectation values of local observables with respect to a MERA, with the same complexity as for the corresponding spin model. This opens up a way to describe fermionic higher-dimensional models without encountering a sign problem. It is the hope that this work stimulates further interest in numerically assessing strongly correlated fermionic models using unitary circuits.

First promising numerical results can be found in Ref. [239]. After finishing this part of the thesis, two other groups presented work on higher-dimensional fermionic systems. Numerics on fermionic MERA were given in Ref. [240] and on fermionic PEPS in Ref. [241]. See Chapter 8 for more details.

8. Contraction of fermionic operator circuits for the simulation of fermionic lattice systems

A fermionic operator circuit is a product of fermionic operators of usually different and partially overlapping support. Further elements of fermionic operator circuits (FOC) are partial traces and partial projections. The presented framework allows for the introduction of fermionic versions of known qudit operator circuits (QUOC), important for the simulation of strongly correlated d -dimensional systems: The multiscale entanglement renormalization ansätze (MERA), tree tensor networks (TTN), projected entangled pair states (PEPS), or their infinite-size versions (iPEPS etc.). After the definition of a FOC, a method is presented that allows for contracting a FOC with the same computation and memory requirements as a corresponding QUOC, for which all fermionic operators are replaced by qudit operators of identical dimension. A given scheme for contracting the qudit circuit relates to an analogous scheme for the corresponding fermionic circuit, where additional marginal computational costs arise only from reordering of modes for operators occurring in intermediate stages of the contraction. This chapter constitutes hence a substantial generalization and improvement of the – perhaps more intuitive – approach of Chap. 7. The results generalize efficient schemes for the simulation of d -dimensional spin systems, as algorithms on MERA, TTN, or PEPS to the fermionic case.

Strongly correlated quantum lattice models pose some of the most intriguing physical questions and technical challenges, due to the fact that the number of degrees of freedom increases exponentially with the system size. Especially for the analysis of ground state properties in one-dimensional systems, the density-matrix renormalization-group (DMRG) [66, 68] provides a numerical approach that is often extraordinarily accurate. It works by variational optimization of a suitable class of states, in this case, the matrix product states [83–85]. For two- and three-dimensional systems, quantum Monte-Carlo methods (e.g., positive-definite path integral [49, 62] or stochastic series expansion [50] representation) are extremely successful for bosonic and unfrustrated spin models, but are bothered by the sign problem [62, 63] for some interesting frustrated spin and fermionic models, including the notorious Fermi-Hubbard model

$$\hat{H} = - \sum_{\langle i,j \rangle, \sigma} (\hat{f}_{i\sigma}^\dagger \hat{f}_{j\sigma} + h.c.) + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} - \mu \sum_{i,\sigma} \hat{n}_{i\sigma}$$

which is a candidate for the description of the essential physics of high-temperature superconductivity. Recently, new tools such as the diagrammatic Monte Carlo method have been developed [53, 242], which have a less severe sign problem and have, e.g., been demonstrated to give precise results for the repulsive Fermi-Hubbard model in the (correlated) Fermi liquid regime [243]; see Secs. 1.1 and 1.2.

In a complementary development, generalizations of DMRG ideas to higher dimensions have been put forward, see Secs. 1.3 and 1.5. To this purpose, first, one needs to give an tensor-contraction ansatz for the many-particle state for which the number of degrees of freedom does only scale polynomial with system size but is (hopefully) still appropriate to describe, e.g., the ground states of the higher-dimensional system. Second, a way of efficiently evaluating interesting local observables or correlators with respect to the ansatz states needs to be identified. Third, a corresponding algorithm to determine or approximate the ground state within the ansatz class on a classical computer needs to be worked out. Focusing first on spin (or equivalently qudit) lattices, several suggestions have been put forward, such as *tensor product ansätze* or *projected entangled pair states* (PEPS) [116–119, 244, 245], *tree tensor networks* (TTN) [246], or *multiscale entanglement renormalization ansätze* (MERA) [120, 125, 231, 128, 129].

This chapter addresses the question of how higher-dimensional *fermionic* systems can be studied via ansatz states. If one maps the system to a spin model by expressing states and operators in the occupation number representation with respect to a fixed ordering of the modes, inevitably long-range ($\mathcal{O}(L^{d-1})$, where L is the linear size of the d -dimensional lattice) interaction terms occur, rendering simulation unfeasible: If one considers, e.g., a term $\hat{f}_j^\dagger \hat{f}_k$, $j < k$, then its spin representation under the Jordan-Wigner transformation [247] is

$$\sigma_j^- \otimes \bigotimes_{j < l < k} \sigma_l^z \otimes \sigma_k^+,$$

containing a so-called Jordan-Wigner string.

Accompanied by first numeric results, fermionic generalizations of MERA states were suggested in Refs. [240, 239] and for PEPS in Ref. [241]. In Chap. 7, an algorithm for fermionic MERA was given that is based on *dynamical reorderings* of fermionic modes; see also Ref. [239]. It exploits the possibility to change the ordering of the fermionic modes during the algorithm to confine all occurring Jordan-Wigner strings to a sublattice of finite extent, the *causal cone* of, e.g., a local observable in the MERA. Going beyond that result, here, the question is posed whether a given general circuit of fermionic operators (FOC, examples in Fig. 8.1) can be contracted with the *same* efficiency as a corresponding circuit of qudit operators (QUOC). This is answered in the affirmative for the case where all operators in the FOC are *parity-symmetric* (either fermion number parity preserving or changing): It is shown constructively that the elementary contraction operations for such a FOC can be executed in an arbitrary sequence and detailed account of the algorithm is given. As compared to the requirements for the contraction of a certain QUOC with a given contraction scheme, the number of operations and memory requirements for the

same contraction scheme, applied to a corresponding FOC, increase only by a marginal amount.

This allows to translate the algorithms already developed for spin systems (for PEPS, e.g., in Refs. [117, 119, 127, 126, 248], for MERA, e.g., in Refs. [125, 229, 128, 129]) to the fermionic case without loss of computational efficiency. Giving further details for the case of PEPS, it is argued that application of the FOC scheme to fermionic PEPS appears to provide a more efficient algorithm than that presented in Ref. [241] where a mapping to a spin system was employed by choice of a fixed mode ordering.

In Sec. 8.1 the idea of the FOC is introduced and it is given a proper definition. Rules for the execution of the elementary contraction operations for two or one operators are derived in Sec. 8.2, after which the importance of a predefined order among the operators constituting the FOC is pointed out in Sec. 8.3. It is also explained how this operator order can be modified with marginal computational cost, allowing to efficiently execute the elementary contractions in an arbitrary sequence. The implications on computational efficiency and locality considerations are summarized in Sec. 8.4. Sec. 8.5 introduces further useful operations on FOCs that are employed in an efficient contraction algorithm for fermionic (i)PEPS in Sec. 8.6. The chapter closes with a short discussion in Sec. 8.7.

8.1. Fermionic operator circuit

8.1.1. General structure

A fermionic operator circuit (FOC) is a product of (not necessarily physical, i.e., in general not particle number parity preserving) fermionic operators $\hat{A}_i : \mathcal{F}_m \rightarrow \mathcal{F}_n$ of in general different support, specified by sets of mode labels $m, n \subset \mathcal{L}$. Further elements of FOCs are partial traces and partial projections. Each mode label $x \in \mathcal{L}$ occurs at most twice, once for an incoming mode of some operator and, the second time, for an outgoing mode of the same or another operator. This means for graphical representations of FOCs as graphs, where each vertex corresponds to one operator $\hat{A}_i$, that each arc (directed edge) of the graph carries a set of unique mode labels. As explained in Sec. 8.1.2 this convention allows for a convenient definition of the FOC such that it has a well-defined value.

Prominent examples of FOCs are fermionic versions of known qudit operator circuits (QUOC), important for the simulation of strongly correlated d -dimensional systems: *multiscale entanglement renormalization ansätze* (MERA) [120] and *tree tensor networks* (TTN) [246]; Fig. 8.1. As shown in Sec. 8.6 also the fermionic variants of *tensor product ansätze* or *projected entangled pair states* (PEPS) [116–119] are covered in the FOC framework; Fig. 8.8. For a MERA, a possible choice for mode labels are the renormalization step τ combined with a site label from the corresponding lattice.

For numerical purposes, each fermionic operator $\hat{A} : \mathcal{F}_m \rightarrow \mathcal{F}_n$ of the circuit is stored in an occupation number representation with respect to certain orderings $\mathbf{m}$ and $\mathbf{n}$ of the sets of modes $m, n \subset \mathcal{L}$. Such orderings are considered as *bijective enumerations* $\mathbf{m} : \{1, \dots, |m|\} \rightarrow m$ and $\mathbf{n} : \{1, \dots, |n|\} \rightarrow n$ of the sets, where $|m|$ denotes the number of elements in m . One may also treat such enumerations as vectors. For a chosen ordering $\mathbf{n}$

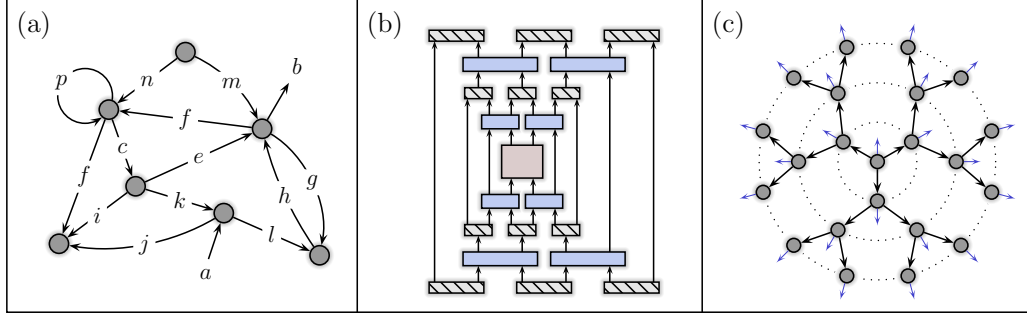


Figure 8.1.: (a) The graphical representation of a FOC as a directed graph. The nodes represent fermionic operators. The arcs (directed edges) represent (partial) multiplications, partial traces, and open indices. Each arc is labeled by the set of modes it corresponds to. The operator corresponding to a certain vertex maps from the modes of all incoming arcs to the modes of the outgoing arcs. In the example, the arc “ e ” corresponds to a partial multiplication, arc “ p ” to a partial trace, and arcs “ a ” and “ b ” to open incoming and outgoing indices, respectively. The node at the top corresponds to a ket vector from $\mathcal{F}_{m \cup n}$ and the node at the bottom left to a bra vector (element of the dual of $\mathcal{F}_{f \cup i \cup j}$). As a whole, the circuit is a fermionic operator mapping from $\mathcal{F}_a$ to $\mathcal{F}_b$.

(b) A FOC for the calculation of the expectation value of a local observable (square in the center) with respect to a MERA state with two renormalization steps. The hatched flat rectangles represent isometries which correspond to a coarse graining step in a (real-space) renormalization procedure. The other rectangles represent unitaries that are supposed to reduce entanglement of adjacent blocks before a coarse graining step. The circuit contains only those unitaries and isometries of the MERA that lie inside the so-called causal cone of the observable; all others cancel out.

(c) FOC for a tree tensor network (TTN) state, here for a genuine tree system, the Bethe lattice with coordination number $z = 3$. To have the value of a FOC well-defined, one needs to specify an ordering among the operators, assigning to each operator a number $\tau = 1, 2, \dots$. In example (a), τ is (arbitrarily) chosen to increase from the bottom to the top. In example (b), a natural ordering, motivated by the picture of subsequent renormalization steps, is also directed from the bottom to the top; as will be explained later, the ordering inside one layer is irrelevant, as the contained isometries are all parity-preserving and operate on disjoint sets of modes. Analogously in example (c), one can choose τ to increase in radial direction, starting from the central node.

of the modes in n , the basis states of the Fock space $\mathcal{F}_n$ are denoted by

$$|\mathbf{n}\rangle_n = |n_1, \dots, n_{|n|}\rangle_n := (\hat{f}_{n_1}^\dagger)^{n_1} \dots (\hat{f}_{n_{|n|}}^\dagger)^{n_{|n|}} |\emptyset\rangle_n, \quad (8.1)$$

where $|\emptyset\rangle_n$ labels the vacuum state of the Fock space $\mathcal{F}_n$ and $\hat{f}_i$ are the corresponding anticommuting ladder operators with $\{\hat{f}_i, \hat{f}_j^\dagger\} = \delta_{ij}$. The operator $\hat{A}$ can hence be stored as the complex $2^{|n|} \times 2^{|m|}$ matrix

$$J_{\mathbf{n},\mathbf{m}}(\hat{A}) = \sum_{\mathbf{n},\mathbf{m}} |\mathbf{n}\rangle_n \langle \mathbf{n} | \hat{A} | \mathbf{m} \rangle_m (\mathbf{m}). \quad (8.2)$$

This is an occupation number representation or Jordan-Wigner transform [247] of the operator $\hat{A}$. Of course it is also possible to restrict (for each set of modes) to a reduced basis. The only information about the basis states actually needed is their particle number parity; see Sec. 8.2.1. The states occurring in (8.2) are elements of different Hilbert spaces: $|\mathbf{m}\rangle_m \in \mathcal{F}_m$, $|\mathbf{n}\rangle_n \in \mathcal{F}_n$, $|\mathbf{m}\rangle \in \mathcal{B}_{|m|}$, and $|\mathbf{n}\rangle \in \mathcal{B}_{|n|}$, where $\mathcal{B}_{|n|}$ denotes the $|n|$ -qubit Hilbert space

$$\mathcal{B}_{|n|} = (\mathbb{C}^2)^{\otimes |n|}. \quad (8.3)$$

A similar approach can be used for anyonic systems [249].

8.1.2. Definition of a FOC

A fermionic operator circuit is specified by a set of fermionic operators $\{\hat{A}_i : \mathcal{F}_m \rightarrow \mathcal{F}_n\}$, where each mode label occurs at most twice, once as an incoming mode of an operator $\hat{A}_i$ and once as an outgoing mode of an operator $\hat{A}_j$. Mode labels which occur two times in this fashion imply a (partial) multiplication, Fig. 8.4a, or (partial) trace, Fig. 8.4b, of the corresponding operators with respect to that set of modes. Both operations together define a general contraction of two operators, namely contraction of some outgoing modes of $\hat{A}$ with some incoming modes of $\hat{B}$ and, simultaneously, of some incoming modes of $\hat{A}$ with some outgoing modes of $\hat{B}$; see Fig. 8.4c. Mode labels, which occur only once, correspond to modes that the FOC as a whole maps from or maps to.

To have the value of a FOC well-defined, one needs to specify an ordering of the contained operators $\{\hat{A}_i\}$. The value of the FOC is then defined by the one resulting from doing the contractions in the order $\hat{A}_N \circ \dots \circ \hat{A}_2 \circ \hat{A}_1$, where “ $\hat{B} \circ \hat{A}$ ” denotes the contraction of all common modes of the operators $\hat{A}$ and $\hat{B}$; see Fig. 8.4c. As discussed in Sec. 8.3, this operation is associative but in general not commutative, $\hat{B} \circ \hat{A} \neq \hat{A} \circ \hat{B}$.

8.1.3. Remarks on the definition

In Sec. 8.2, as for the partial contraction operation, also a rule for a partial projection of some modes to basis states (i.e., $\{\hat{n}_i\}$ eigenstates) will be given. This is actually already covered by the contraction operation but perhaps useful to have explicitly, as such projections are frequently used in considerations on operator circuits.

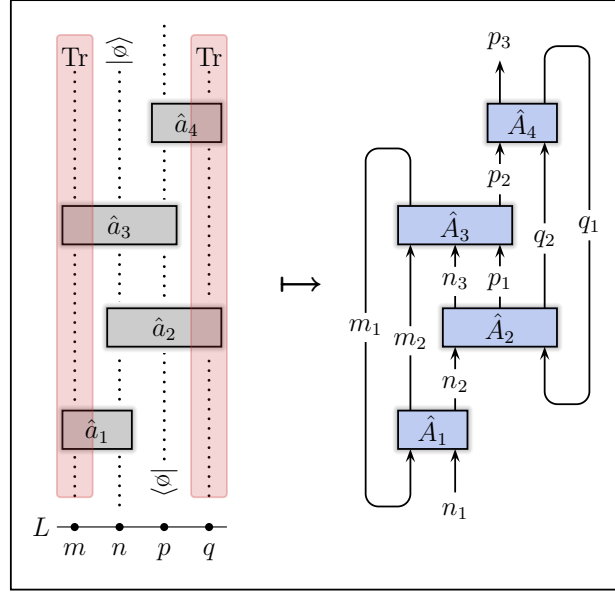


Figure 8.2.: The operator order goes from the bottom to the top. Left: Example for an operator circuit on a lattice $L = m \cup n \cup p \cup q$. It corresponds to the expression $\text{Tr}_{m \cup q}({}_n \langle \emptyset | \hat{A}_4 \cdot \dots \cdot \hat{A}_1 | \emptyset \rangle_p)$, cmp. Eq. (8.4), where, e.g., $\hat{A}_1 = \hat{a}_1 \otimes \text{Id}_{p \cup q}$. For convenience, the definition of fermionic operator circuits, Sec. 8.1.2, requires that each mode occurs at most twice, once as an incoming mode and once as an outgoing mode of some operators. This can be achieved by a relabeling of the modes, yielding the FOC $\hat{A}_4 \circ \dots \circ \hat{A}_1$ (right). This does not change the matrix elements of the operators and the FOC. One has for example ${}_{m^{(2)} \oplus n^{(2)}} \langle m' n' | \hat{A}_1 | m n \rangle_{m^{(1)} \oplus n^{(1)}} = {}_{m \oplus n} \langle m' n' | \hat{a}_1 | m n \rangle_{m \oplus n}$, where m , n , $m^{(i)}$, $n^{(i)}$ are orderings of the sets of modes m , n , m_i , and n_i . Here, with the relabeling, also the partial projections for operators $\hat{a}_2$ and $\hat{a}_3$ have been executed.

Note that the operators $\{\hat{A}_i\}$ are not assumed to be from the so-called algebra of physical operators – i.e., particle number parity preserving. This is for example useful when calculating correlators of the form $\langle \hat{f}_i^\dagger \hat{f}_j \rangle$ with respect to MERA or TTN states. In such a calculation, the operators $\hat{f}_i^\dagger$ and $\hat{f}_j$ become (clearly not parity preserving) elements of a FOC.

However, it will be explained in Sec. 8.3 that in order to be able to do the contraction of the FOC in an arbitrary sequence (necessary to get optimum numerical efficiency), i.e., to be able to deviate from the order $\hat{A}_N \circ \dots \circ \hat{A}_2 \circ \hat{A}_1$, it is in general necessary that each $\hat{A}_i$ is either parity preserving or parity changing.

That mode labels are required to be unique is not a limitation. Consider for example an

operator circuit that is defined on a lattice L and does not have that property,

$$\text{Tr}_t(\text{ }_o\langle\emptyset|\hat{\mathcal{A}}_N \cdot \dots \cdot \hat{\mathcal{A}}_2 \cdot \hat{\mathcal{A}}_1|\emptyset\rangle_i). \quad (8.4)$$

Here $t \subset L$ denotes a subset of modes that are traced out, and i and $o \subset L$ denote subsets of modes that are projected out; $t \cap (i \cup o) = \emptyset$. The circuit hence maps from $\mathcal{F}_{L \setminus (t \cup i)}$ to $\mathcal{F}_{L \setminus (t \cup o)}$. Each operator $\hat{\mathcal{A}}_i$ acts nontrivially on a subset of the modes: $\hat{\mathcal{A}}_i = \hat{a}_i \otimes \text{Id}_{L \setminus \ell_i}$ with $\hat{a}_i : \mathcal{F}_{\ell_i} \rightarrow \mathcal{F}_{\ell_i}$ where $\ell_i \subset L$. Now, relabeling of the modes to make the modes unique as depicted in Fig. 8.2, does of course not change the matrix elements of the FOC. It yields a proper FOC $\hat{A}_N \circ \dots \circ \hat{A}_2 \circ \hat{A}_1$, where each operator $\hat{A}_i$ has the same matrix elements as the corresponding $\hat{a}_i$ (partial projections onto the vacuum can be executed in the same step, as in our example, or introduced as separate elements of the FOC). The contraction rules in Sec. 8.2 are constructed such that this FOC and (8.4) have the same matrix elements, i.e., are related by a trivial relabeling of incoming and outgoing modes.

8.1.4. Rationale behind calculations and derivations

- The fermionic operators are maps from one Fock space of “incoming modes” to another (in general unrelated) Fock space of “outgoing modes”. In general, they are of different dimension.
- Each arc (directed edge) in a graphical representation of a FOC corresponds to a set of unique fermionic modes.
- Vacuum states are mode specific. Ladder operators of other unrelated modes commute with the vacuum state for other modes. Take for example $n = \{1, 2\}$ and $\mathbf{n} = (1, 2)$, then

$$\begin{aligned} \hat{f}_3^\dagger |n_1 n_2\rangle_{\mathbf{n}} &= \hat{f}_3^\dagger (\hat{f}_1^\dagger)^{n_1} (\hat{f}_2^\dagger)^{n_2} |\emptyset\rangle_n \\ &= (-1)^{n_1+n_2} (\hat{f}_1^\dagger)^{n_1} (\hat{f}_2^\dagger)^{n_2} |\emptyset\rangle_n \cdot \hat{f}_3^\dagger \\ &= (-1)^{n_1+n_2} |n_1 n_2\rangle_{\mathbf{n}} \cdot \hat{f}_3^\dagger \end{aligned} \quad (8.5)$$

The rationale behind this is that if one has an expression ${}_m \cup n \langle \emptyset | \hat{A}_m \hat{A}_n | \emptyset \rangle_{{}_m \cup n}$ for disjoint sets of modes m and n , and where $\hat{A}_m$ and $\hat{A}_n$ are polynomials in the ladder operators of the modes in m and n , respectively, it evaluates to

$${}_n \langle \emptyset | {}_m \langle \emptyset | \hat{A}_m \hat{A}_n | \emptyset \rangle_m | \emptyset \rangle_n = {}_m \langle \emptyset | \hat{A}_m | \emptyset \rangle_m {}_n \langle \emptyset | \hat{A}_n | \emptyset \rangle_n.$$

8.1.5. Notation

The Einstein summation convention is employed, i.e., basis state labels that occur twice in an expression presuppose summation over that basis.

Basis states for a certain set $m \subset \mathcal{L}$ of $|m|$ fermionic modes and an ordering $\mathbf{m}$ of those modes will be denoted by $|\mathbf{m}\rangle_{\mathbf{m}} = (\hat{F}_{\mathbf{m}}^{\mathbf{m}})^{\dagger}|\emptyset\rangle_{\mathbf{m}}$, where $\mathbf{m} \in \{0, 1\}^{|m|}$ and

$$\hat{F}_{\mathbf{m}}^{\mathbf{m}} := (\hat{f}_{\mathbf{m}_{|m|}})^{m_{|m|}} \cdot \dots \cdot (\hat{f}_{\mathbf{m}_2})^{m_2} (\hat{f}_{\mathbf{m}_1})^{m_1}.$$

The number of particles in a basis state $|\mathbf{m}\rangle_{\mathbf{m}}$ is denominated by

$$\bar{m} := \sum_i m_i. \quad (8.6)$$

The parity of the basis state is $(-1)^{\bar{m}}$.

Whenever references to Fock spaces for unions of sets of modes occur, as in $\mathcal{F}_{m \cup n}$, it is implied that those sets of modes are disjoint, i.e., $m \cap n = \emptyset$ in that case.

With $\hat{B} \cdot_n \hat{A}$, a partial multiplication is denoted. Only the outgoing modes n of $\hat{A}$ are contracted with the corresponding same incoming modes n of $\hat{B}$. Correspondingly $\text{Tr}_r \hat{B}$ denotes a partial trace, the contraction of incoming modes r with outgoing modes r . The expression $\hat{B} \circ \hat{A}$ denotes a (partial) contraction of all common incoming/outgoing modes of $\hat{A}$ with corresponding outgoing/incoming modes of $\hat{B}$.

8.2. Contractions

In the following, rules are given for all elementary contraction operations needed during the evaluation of a FOC. No non-local Jordan-Wigner transformations occur. The only reordering of modes necessary is for incoming or outgoing modes of single operators, directly before a partial multiplication, trace etc. that they are affected by.

8.2.1. Reordering of modes

Assume we are given a fermionic operator $\hat{A} : \mathcal{F}_m \rightarrow \mathcal{F}_n$ in the occupation number representation $J_{\mathbf{n}, \mathbf{m}}(\hat{A})$. The contraction rules to follow, will pose some preconditions on the orderings of modes (to get simple formulae). One needs hence to be able to derive from $J_{\mathbf{n}, \mathbf{m}}(\hat{A})$ representations $J_{\mathbf{n}', \mathbf{m}'}(\hat{A})$ with different mode orders.

All reorderings can be written as sequences of two mode swaps. Let us assume that $\mathbf{m}' = \mathbf{m}$ and that orderings $\mathbf{n}$ and $\mathbf{n}'$ differ only in modes $\mathbf{n}_j$ and $\mathbf{n}_k$ (for $1 \leq j < k \leq |n|$), i.e., $\mathbf{n}'_j = \mathbf{n}_k$ and $\mathbf{n}'_k = \mathbf{n}_j$. Where in the old representation, $|\mathbf{n}\rangle$ corresponds to the state $|\mathbf{n}\rangle_{\mathbf{n}} = (\hat{f}_{\mathbf{n}_1})^{n_1} \dots (\hat{f}_{\mathbf{n}_j})^{n_j} \dots (\hat{f}_{\mathbf{n}_k})^{n_k} \dots |\emptyset\rangle_{\mathbf{n}}$, it corresponds in the new representation to $|\mathbf{n}\rangle_{\mathbf{n}'} = (\hat{f}_{\mathbf{n}_1})^{n_1} \dots (\hat{f}_{\mathbf{n}_k})^{n_j} \dots (\hat{f}_{\mathbf{n}_j})^{n_k} \dots |\emptyset\rangle_{\mathbf{n}}$.

To derive the corresponding transformation on the representations of $\hat{A}$, note that an operator $\hat{S}_{jk}$ that swaps the modes, i.e., $\hat{S}_{jk} \hat{f}_j \hat{S}_{jk}^{\dagger} = \hat{f}_k$ and $\hat{S}_{jk} \hat{f}_k \hat{S}_{jk}^{\dagger} = \hat{f}_j$ is given by [236]

$$\hat{S}_{jk} = \mathbb{1} - \hat{f}_j^{\dagger} \hat{f}_j - \hat{f}_k^{\dagger} \hat{f}_k + \hat{f}_j^{\dagger} \hat{f}_k + \hat{f}_k^{\dagger} \hat{f}_j. \quad (8.7)$$

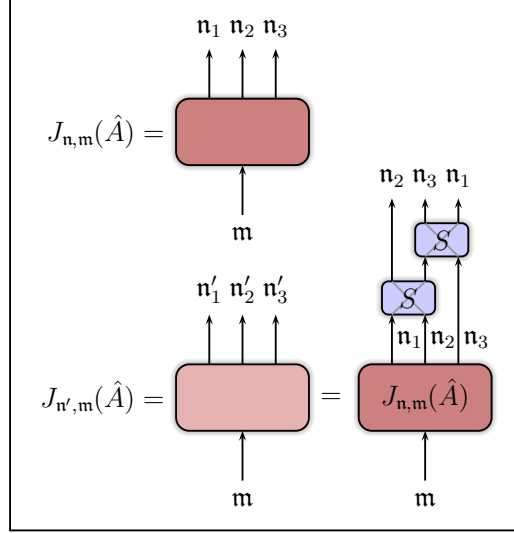


Figure 8.3.: To implement contraction schemes for FOCs on a computer, every operator $\hat{A} : \mathcal{F}_m \rightarrow \mathcal{F}_n$ is stored in an occupation number representation $J_{n,m}(\hat{A})$. The primitive contraction rules, given in Sec. 8.2, pose some preconditions on the orderings of modes (to get simple formulae). Hence, before applying those rules, it is in general necessary to change, e.g., from $J_{n,m}(\hat{A})$ to a representation $J_{n',m'}(\hat{A})$ with different mode ordering. In the depicted example, the order of the outgoing modes changes from $\mathbf{n} = (n_1, n_2, n_3)$ to $\mathbf{n}' = (n_2, n_3, n_1)$. As explained in Sec. 8.2.1, this requires application of the swap matrix S [Eq. (8.9)] – in this example two times.

With $\hat{S}_{jk}|\emptyset\rangle_n = |\emptyset\rangle_n$, one has hence

$$J_{n',m}(\hat{A}) = J_{n,m}(\hat{S}_{jk}\hat{A}) = J_{n,n}(\hat{S}_{jk})J_{n,m}(\hat{A}) \quad (8.8)$$

The occupation number representation (Jordan-Wigner transform) of a term $\hat{f}_j^\dagger \hat{f}_k$ is $\sigma_j^- \otimes (\bigotimes_{l=j+1}^{k-1} \sigma_l^z) \otimes \sigma_k^+$, where the σ^α denote the Pauli matrices. The swap operator for two consecutive modes is in the relevant subspace

$$\begin{aligned} S &:= J_{(i,i+1),(i,i+1)}(\hat{S}_{i,i+1}) \\ &= |0,0\rangle\langle 0,0| - |1,1\rangle\langle 1,1| \\ &\quad + |0,1\rangle\langle 1,0| + |1,0\rangle\langle 0,1|. \end{aligned} \quad (8.9)$$

In practice one may choose to execute all mode reorderings by application of corresponding sequences of swap operators for consecutive modes; see Fig. 8.3.

Swapping of whole sets of modes, e.g., useful when retaining reduced bases, can be done as well. Consider an operator $\hat{B} : \mathcal{F}_m \rightarrow \mathcal{F}_{u \cup v \cup x \cup z}$ given in the representation $J_{\mathbf{n},m}(\hat{B})$ with $\mathbf{n} = \mathbf{u} \oplus \mathbf{v} \oplus \mathbf{x} \oplus \mathbf{z}$ where $\mathbf{u}, \mathbf{v}, \mathbf{x}, \mathbf{z}$ are orderings for the modes in u, v, x , and

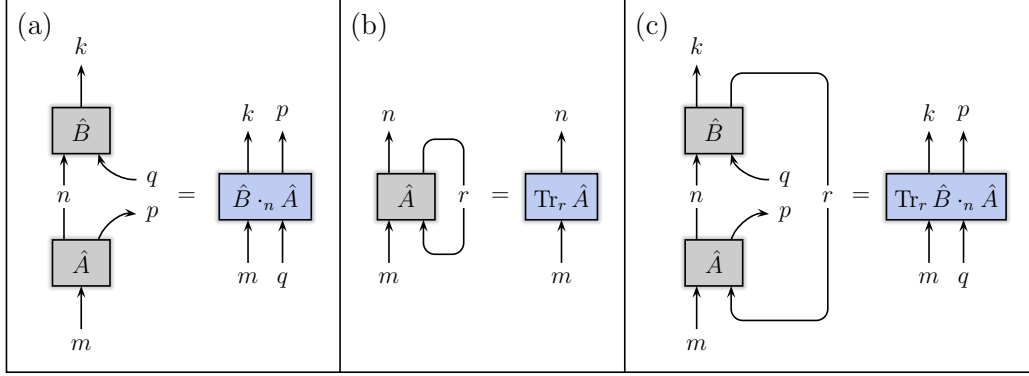


Figure 8.4.: Listing of all (contraction) operations that are needed to evaluate a FOC: (a) partial multiplication $\hat{B} \cdot_n \hat{A}$, (b) partial trace $\text{Tr}_r \hat{A}$, (c) partial contraction $\hat{B} \circ \hat{A} = \text{Tr}_r \hat{B} \cdot_n \hat{A}$. The latter is not a primitive operation, but rather a combination of operations (a) and (b). In all cases, the lower operator is defined to come first in the operator ordering.

z . Swapping $\mathfrak{v}$ and $\mathfrak{x}$, is achieved by $(\mathbf{u}\mathbf{x}\mathbf{v}\mathbf{z}|J_{\mathfrak{n}',\mathfrak{m}}(\hat{B})|\mathbf{m}) = (-1)^{\bar{x}\bar{v}}(\mathbf{u}\mathbf{v}\mathbf{x}\mathbf{z}|J_{\mathfrak{n},\mathfrak{m}}(\hat{B})|\mathbf{m})$, where $\mathfrak{n}' = \mathfrak{u} \oplus \mathfrak{x} \oplus \mathfrak{v} \oplus \mathfrak{z}$.

8.2.2. Contraction of some outgoing modes of $\hat{A}$ with the corresponding incoming modes of $\hat{B}$

The partial multiplication of two operators is depicted in Fig. 8.4a. Let $\hat{A} : \mathcal{F}_m \rightarrow \mathcal{F}_{n \cup p}$ and $\hat{B} : \mathcal{F}_{n \cup q} \rightarrow \mathcal{F}_k$, i.e., the operators' outgoing/incoming supports overlap in the modes n . Let $\mathfrak{m}$, $\mathfrak{n}$, $\mathfrak{p}$, and $\mathfrak{q}$ be orderings for the modes in m , n , p , and q . Assuming we have the two operators in representations $A = J_{\mathfrak{a},\mathfrak{m}}(\hat{A})$ and $B = J_{\mathfrak{k},\mathfrak{b}}(\hat{B})$ with $\mathfrak{a} = \mathfrak{n} \oplus \mathfrak{p}$ and $\mathfrak{b} = \mathfrak{n} \oplus \mathfrak{q}$, the resulting operator $\hat{C} := \hat{B} \cdot_n \hat{A} : \mathcal{F}_{m \cup q} \rightarrow \mathcal{F}_{k \cup p}$ with orderings $\mathfrak{c}_1 = \mathfrak{k} \oplus \mathfrak{p}$, $\mathfrak{c}_2 = \mathfrak{m} \oplus \mathfrak{q}$ is

$$\begin{aligned}
 \hat{C} &= \hat{B} \cdot_n \hat{A} \\
 &= |\mathbf{k}\rangle_{\mathfrak{k}} (\mathbf{k}|B|\mathbf{n}'\mathbf{q})_{\mathfrak{b}} \langle \mathbf{n}'\mathbf{q}| \cdot |\mathbf{np}\rangle_{\mathfrak{a}} (\mathbf{np}|A|\mathbf{m})_{\mathfrak{m}} \langle \mathbf{m}| \\
 &= (-1)^{\bar{p}\bar{q} + (\bar{p} + \bar{q})(\bar{n} + \bar{n}')} |\mathbf{k}\rangle_{\mathfrak{k}} (\mathbf{k}|B|\mathbf{n}'\mathbf{q}) \\
 &\quad \times {}_q \langle \emptyset | {}_n \langle \emptyset | (F_{\mathfrak{p}}^{\mathfrak{p}})^{\dagger} F_{\mathfrak{n}}^{\mathfrak{n}'} (F_{\mathfrak{n}}^{\mathfrak{n}})^{\dagger} F_{\mathfrak{q}}^{\mathfrak{q}} |\emptyset\rangle_n |\emptyset\rangle_p \\
 &\quad \times (\mathbf{np}|A|\mathbf{m})_{\mathfrak{m}} \langle \mathbf{m}| \\
 &= (-1)^{\bar{p}\bar{q}} \cdot |\mathbf{kp}\rangle_{\mathfrak{c}_1} (\mathbf{k}|B|\mathbf{nq})(\mathbf{np}|A|\mathbf{m})_{\mathfrak{c}_2} \langle \mathbf{mq}| \\
 &=: |\mathbf{kp}\rangle_{\mathfrak{c}_1} (\mathbf{kp}|C|\mathbf{mq})_{\mathfrak{c}_2} \langle \mathbf{mq}|,
 \end{aligned} \tag{8.10}$$

where C is the representation $C = J_{\mathfrak{c}_1, \mathfrak{c}_2}(\hat{C})$. In short, the transformation rule for the occupation number representations reads

$$(\mathbf{kp}|C|\mathbf{mq}) = (-1)^{\bar{p}\bar{q}} (\mathbf{k}|B|\mathbf{nq})(\mathbf{np}|A|\mathbf{m}). \tag{8.11}$$

In appendix 8.8, an alternative derivation of this rule is given, where the support of operators $\hat{A}$ and $\hat{B}$ is extended prior to the contraction such that there is no need for applying the commutation prescription (8.5). The result is the same.

8.2.3. Partial trace of an operator

The partial trace of an operator is depicted in Fig. 8.4b. Let $\hat{A} : \mathcal{F}_{m \cup r} \rightarrow \mathcal{F}_{n \cup r}$ i.e., the operator's outgoing and incoming supports overlap in the modes r . Such operators can always be decomposed in the form

$$\hat{A} = \hat{A}_+ + \hat{A}_-, \quad (8.12)$$

where $\hat{A}_+$ is the particle number parity preserving and $\hat{A}_-$ the parity changing component, i.e.,

$$(-1)^{\hat{N}_n + \hat{N}_r} \hat{A}_\pm = \pm \hat{A}_\pm (-1)^{\hat{N}_m + \hat{N}_r} \quad (8.13)$$

with $\hat{N}_r := \sum_{i \in r} \hat{f}_i^\dagger \hat{f}_i$.

The correct expression for the partial trace follows from its defining property that $\text{Tr}(\hat{A}\hat{B}) = \text{Tr}(\text{Tr}_r(\hat{A})\hat{B})$ for all operators $\hat{B}$ that have no support on modes r . Hence, let us consider such an operator $\hat{B} : \mathcal{F}_{n \cup r} \rightarrow \mathcal{F}_{m \cup r}$ with no support on r , i.e., $\hat{f}_i \hat{B}_\pm = \pm \hat{B}_\pm \hat{f}_i \forall i \in r$. Let $\mathfrak{m}, \mathfrak{n}, \mathfrak{r}$ be orderings for the modes in m, n , and r . Further let $\mathfrak{a} = \mathfrak{m} \oplus \mathfrak{r}$ and $\mathfrak{b} = \mathfrak{n} \oplus \mathfrak{r}$. The operator's matrix elements obey

$$\begin{aligned} & {}_{\mathfrak{a}}\langle \mathfrak{m} \mathfrak{r}' | \hat{B} | \mathfrak{n} \mathfrak{r} \rangle_{\mathfrak{b}} \\ &= {}_{\mathfrak{a}}\langle \emptyset | \hat{F}_{\mathfrak{r}}^{\mathfrak{r}'} \hat{F}_{\mathfrak{m}}^{\mathfrak{m}} \hat{B} (\hat{F}_{\mathfrak{n}}^{\mathfrak{n}})^\dagger (\hat{F}_{\mathfrak{r}}^{\mathfrak{r}})^\dagger | \emptyset \rangle_{\mathfrak{b}} \\ &= (-1)^{\bar{r}'\bar{m} + \bar{r}\bar{n}} {}_{\mathfrak{m}}\langle \emptyset | {}_r\langle \emptyset | \hat{F}_{\mathfrak{m}}^{\mathfrak{m}} \hat{F}_{\mathfrak{r}}^{\mathfrak{r}'} \hat{B} (\hat{F}_{\mathfrak{r}}^{\mathfrak{r}})^\dagger (\hat{F}_{\mathfrak{n}}^{\mathfrak{n}})^\dagger | \emptyset \rangle_r | \emptyset \rangle_{\mathfrak{n}} \\ &= \delta_{\mathfrak{r}\mathfrak{r}'} (-1)^{\bar{r}(\bar{m} + \bar{n})} {}_{\mathfrak{m}}\langle \mathfrak{m} | \hat{B}_+ + (-1)^{\bar{r}} \hat{B}_- | \mathfrak{n} \rangle_{\mathfrak{n}} \\ &= \delta_{\mathfrak{r}\mathfrak{r}'} {}_{\mathfrak{m}}\langle \mathfrak{m} | \hat{B} | \mathfrak{n} \rangle_{\mathfrak{n}}. \end{aligned} \quad (8.14)$$

Requiring that

$$\text{Tr}(\hat{A}\hat{B}) = {}_{\mathfrak{b}}\langle \mathfrak{n} \mathfrak{r} | \hat{A} | \mathfrak{m} \mathfrak{r} \rangle_{\mathfrak{a}} {}_{\mathfrak{m}}\langle \mathfrak{m} | \hat{B} | \mathfrak{n} \rangle_{\mathfrak{n}} = \text{Tr}((\text{Tr}_r \hat{A})\hat{B}),$$

is true for all operators $\hat{B}$ with the properties stated above, leads to the conclusion that the partial trace for the modes r is simply given by the expression

$$\text{Tr}_r \hat{A} = \sum_{\mathfrak{r}} |\mathfrak{n} \rangle_{\mathfrak{n}} {}_{\mathfrak{b}}\langle \mathfrak{n} \mathfrak{r} | \hat{A} | \mathfrak{m} \mathfrak{r} \rangle_{\mathfrak{a}} {}_{\mathfrak{m}}\langle \mathfrak{m} |. \quad (8.15)$$

Hence, assuming we have the operator in the representation $J_{\mathfrak{b},\mathfrak{a}}(\hat{A})$, the resulting operator $\text{Tr}_r \hat{A} : \mathcal{F}_{\mathfrak{m}} \rightarrow \mathcal{F}_{\mathfrak{n}}$ is in the occupation number representation

$$(\mathfrak{n} | J_{\mathfrak{n},\mathfrak{m}}(\text{Tr}_r \hat{A}) | \mathfrak{m}) = (\mathfrak{n} \mathfrak{r} | J_{\mathfrak{b},\mathfrak{a}}(\hat{A}) | \mathfrak{m} \mathfrak{r}). \quad (8.16)$$

Please note that the orderings of the modes has been chosen such that, in Eq. (8.14), two sign factors compensate – that of a mode reordering with one from commuting $\hat{F}_\tau^r$ and the operator $\hat{B}$. A sign factor $(-1)^{\bar{r}(\bar{m}+\bar{n})}$ would occur in the expressions for the partial trace, had we swapped the order of $\mathfrak{m}$ ($\mathfrak{n}$) and τ in the ordering of the incoming (outgoing) modes, i.e., $\mathfrak{a} = \tau \oplus \mathfrak{m}$ ($\mathfrak{b} = \tau \oplus \mathfrak{n}$) instead of our choice here. For such a case, the preparative mode reordering would take account of the sign factor and then, having realized the preconditions of it, one would apply rule (8.16).

8.2.4. Contraction of some outgoing modes of $\hat{A}$ with the corresponding incoming modes of $\hat{B}$ and vice versa

Combining partial multiplication (8.10) with partial trace (8.15) one obtains a general partial contraction, namely, that of some outgoing modes n of operator $\hat{A}$ with the corresponding incoming modes of $\hat{B}$ and, simultaneously, contraction of some outgoing modes r of $\hat{B}$ with the corresponding incoming modes of $\hat{A}$. This corresponds to the partial contraction depicted in Fig. 8.4c.

Let $\hat{A} : \mathcal{F}_{m \cup r} \rightarrow \mathcal{F}_{n \cup p}$ and $\hat{B} : \mathcal{F}_{n \cup q} \rightarrow \mathcal{F}_{k \cup r}$, i.e., the operators outgoing/incoming supports overlap in the modes n and r . Let $\mathfrak{m}, \mathfrak{n}, \tau, \mathfrak{p}, \mathfrak{q}, \mathfrak{k}$ be orderings for the modes in m, n, r, p, q , and k . Assuming we have the two operators in representations $A = J_{\mathfrak{n} \oplus \mathfrak{p}, \mathfrak{m} \oplus \tau}(\hat{A})$ and $B = J_{\mathfrak{k} \oplus \tau, \mathfrak{n} \oplus \mathfrak{q}}(\hat{B})$, with $\mathfrak{a} = \mathfrak{k} \oplus \mathfrak{p}$ and $\mathfrak{b} = \mathfrak{m} \oplus \mathfrak{q}$, the resulting operator $\hat{C} : \mathcal{F}_{m \cup q} \rightarrow \mathcal{F}_{k \cup p}$ is

$$\begin{aligned} \hat{C} &= \text{Tr}_r \hat{B} \cdot_n \hat{A} \\ &= (-1)^{\bar{p}\bar{q} + \bar{r}(\bar{p} + \bar{q})} \cdot |kp\rangle_{\mathfrak{a}} (kr|B|nq)(np|A|mr)_{\mathfrak{b}} \langle mq|, \end{aligned}$$

i.e.,

$$\begin{aligned} (kp|J_{\mathfrak{a}, \mathfrak{b}}(\hat{C})|mq) \\ = (-1)^{\bar{p}\bar{q} + \bar{r}(\bar{p} + \bar{q})} \cdot (kr|B|nq)(np|A|mr). \end{aligned} \quad (8.17)$$

In the following, $\hat{B} \circ \hat{A}$ denotes a (partial) contraction of all common incoming/outgoing modes of $\hat{A}$ with corresponding outgoing/incoming modes of $\hat{B}$ according to Eq. (8.17).

8.2.5. Partial projection

The partial projection for an operator is not a new primitive. It is actually an application of the partial multiplication. It is however useful to give it explicitly as partial projections are frequently used in considerations about operator circuits. Let $\hat{A} : \mathcal{F}_m \rightarrow \mathcal{F}_{r \cup n}$. Let $\tau, \mathfrak{m}, \mathfrak{n}$ be orderings for the modes in r, m , and n . Further let $\mathfrak{a} = \tau \oplus \mathfrak{n}$. After projection of modes r onto a basis state $(\{\hat{n}_i\}_{i \in r} \text{ eigenstate}) |r'\rangle_{\tau} = (\hat{F}_{\tau}^{r'})^{\dagger} |\emptyset\rangle_r$, the resulting operator $\hat{A}' : \mathcal{F}_m \rightarrow \mathcal{F}_n$ is

$$\begin{aligned} \hat{A}' &= {}_{\tau} \langle r' | \cdot |rn\rangle_{\mathfrak{a}} (rn|J_{\mathfrak{a}, \mathfrak{m}}(\hat{A})|m)_{\mathfrak{m}} \langle m| \\ &= |n\rangle_{\mathfrak{n}} (r'n|J_{\mathfrak{a}, \mathfrak{m}}(\hat{A})|m)_{\mathfrak{m}} \langle m|, \end{aligned} \quad (8.18)$$

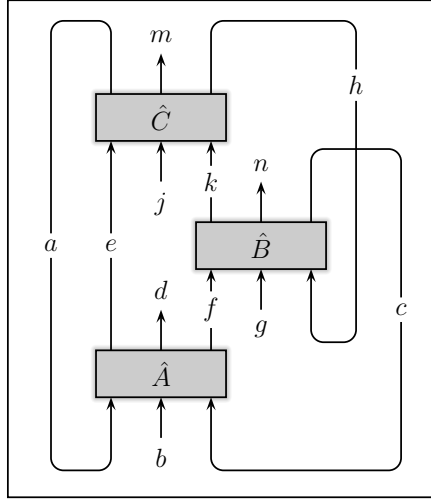


Figure 8.5.: The most general FOC with three operators. To verify that the contraction of operators as given by rule (8.17) is associative, one needs to compare the results of $\hat{C} \circ (\hat{B} \circ \hat{A})$ and $(\hat{C} \circ \hat{B}) \circ \hat{A}$. Both do indeed agree.

i.e.,

$$(n|J_{n,m}(\hat{A}')|m) = (r'n|J_{a,m}(\hat{A})|m). \quad (8.19)$$

A sign factor $(-1)^{r'n}$ would occur, if we would swap the order of modes r and n in the order a of the outgoing modes.

8.3. Operator order and contraction sequence

In Sec. 8.1.2, the value of the FOC was defined as the value resulting from executing the contractions of the constituting operators $\hat{A}_i$ with respect to a certain operator order, $\hat{A}_N \circ \dots \circ \hat{A}_2 \circ \hat{A}_1$. This definition is only sufficient if the contraction (8.17) of operators, as depicted in Fig. 8.4c, is indeed associative. For the most general FOC of three operators $\hat{A} : \mathcal{F}_{aUbUc} \rightarrow \mathcal{F}_{dUeUf}$, $\hat{B} : \mathcal{F}_{fUgUh} \rightarrow \mathcal{F}_{cUkUn}$, and $\hat{C} : \mathcal{F}_{eUjUk} \rightarrow \mathcal{F}_{aUhUm}$ one finds indeed (see Fig. 8.5)

$$\hat{C} \circ (\hat{B} \circ \hat{A}) = (\hat{C} \circ \hat{B}) \circ \hat{A}, \quad (8.20)$$

confirming the consistency of the contraction rule (8.17).

Numerically it may be more efficient to execute for example first the contraction between $\hat{A}_1$ and $\hat{A}_3$ and contract the result with $\hat{A}_2$ afterwards. To be able to choose an arbitrary sequence for the contractions as is possible for the corresponding QUOCs, one needs to be able to change the ordering of the operators without changing the value of the FOC. In the elementary contractions, the ordering of the affected operators matters,

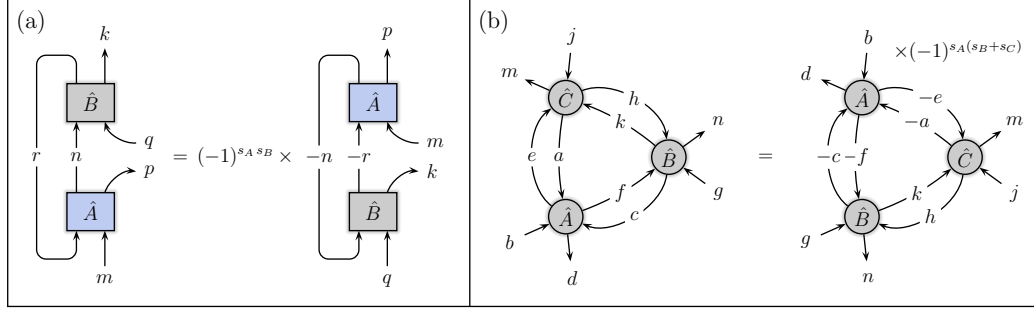


Figure 8.6.: To allow for arbitrary contraction sequences, one needs to be able to change the operator ordering. In the diagrams, the operator order is defined to increase from the bottom to the top. If all operators are parity-symmetric (either preserve or change the fermion number parity; $s = 0$ or $s = 1$), swapping of operators can be done and the resulting sign factors taken account of efficiently. (a) The generic rule (8.21) for swapping two operators that are neighbors in the ordering. (b) An Identity for the most generic FOC with three operators, the same as in Fig. 8.5, depicted in a slightly different fashion. A minus sign at the contraction arc for a mode set n indicates that a sign factor $(-1)^{\bar{n}}$ is to be inserted in the contraction formula (see text).

i.e., for two operators $\hat{A} : \mathcal{F}_{m \cup r} \rightarrow \mathcal{F}_{n \cup p}$ and $\hat{B} : \mathcal{F}_{n \cup q} \rightarrow \mathcal{F}_{k \cup r}$, one has in general $\text{Tr}_r \hat{B} \cdot_n \hat{A} \neq \text{Tr}_n \hat{A} \cdot_r \hat{B}$. However, if each of the two operators is either parity preserving ($s = 0$) or parity changing ($s = 1$), one finds the simple relation

$$\text{Tr}_r \hat{B} \cdot_n \hat{A} = (-1)^{s_A s_B} \text{Tr}_n[(\hat{P}_n \cdot_n \hat{A} \cdot_r \hat{P}_r) \cdot_r \hat{B}], \quad (8.21)$$

where $\hat{P}_n : \mathcal{F}_n \rightarrow \mathcal{F}_n$ with ${}_n \langle \mathbf{n}' | \hat{P}_n | \mathbf{n} \rangle_n = \delta_{\mathbf{n} \mathbf{n}'} (-1)^{\bar{n}}$. In the more compact notation this reads $\hat{B} \circ \hat{A} = (-1)^{s_A s_B} \hat{P}_n \circ \hat{A} \circ \hat{P}_r \circ \hat{B}$. In an implementation, instead of inserting the $\hat{P}_n$ in this fashion as operators or applying them directly to $\hat{A}$ or $\hat{B}$, more efficiently, one may introduce a binary counter (with initial state 0) for each contraction arc – in this case, for the contraction with respect to modes n . Whenever a factor $\hat{P}_n$ arises when swapping the order of operators that have both support on n , the state of the binary counter is inverted. Once, the contraction with respect to modes n is executed, one inserts the factor $(-1)^{\bar{n}}$ in the corresponding expression, if the state of the counter is 1. In the graphical representation of a FOC, the state 1 of the counter is denoted by a minus sign at the corresponding contraction arc as exemplified in Fig. 8.6. The numerical overhead for keeping track of those signs is marginal.

In the following, operators $\hat{A} : \mathcal{F}_m \rightarrow \mathcal{F}_n$ that are either fermion number parity preserving or changing,

$$(-1)^{\hat{N}_n} \hat{A} = \pm \hat{A} (-1)^{\hat{N}_m}, \quad (8.22)$$

are called *parity-symmetric*. Also FOCs that contain only parity-symmetric operators are called parity-symmetric.

Using the above result, it is possible to do the operator contractions of a parity-symmetric FOC in an arbitrary sequence. One starts with the predefined operator order. To execute the contraction of two (arbitrary) operators of the FOC:

- Apply rule (8.21) to bring the two operators into direct neighborhood in the operator order, keeping track of the resulting sign factors for the contraction arcs and of the global sign,
- apply mode swapping operators as described in Sec. 8.2.1, to bring the occupation number representations of the two operators into accord with the precondition of the general contraction rule (8.17), and
- replace the two operators by their contraction according to the rule (8.17).

Consequently, the contraction of a FOC can be done efficiently – with the same sequence of partial contractions as for a corresponding qudit operator circuit. No non-local Jordan-Wigner transformations occur. Marginal computational overheads result from keeping track of certain sign factors when doing contractions in a sequence that deviates from the ordering of the circuit’s operators and reordering of modes for incoming or outgoing modes of single operators, directly before a partial multiplication, trace etc. that they are affected by.

The operator order is part of the definition of a FOC. For the example of the fermionic MERA it can be chosen to agree with the physical interpretation as consecutive renormalization steps; i.e., the operator order is increasing with the renormalization number. As all unitaries (isometries) of a particular renormalization stage commute, the ordering among those can be chosen arbitrarily. In Sec. 8.6 a useful operator ordering for fermionic PEPS is presented.

8.4. Computational costs and locality

Given a contraction sequence for a qudit operator circuit (QUOC), the same sequence can be used for a corresponding parity-symmetric FOC (for which all qudit operators are replaced by parity-symmetric fermionic operators of identical dimension). There is hence no memory or computational overhead *per se*. For the elementary contraction operations stated in Sec. 8.2, a certain ordering of the modes was being assumed, prior to the operation. If one uses the contraction operations as stated there, one gets a marginal overhead from the corresponding preparative mode reorderings; Sec. 8.2.1. The number of numerical operations needed for a reordering is proportional to the size of the operator matrix: every reordering can be achieved by a sequence of swaps of consecutive modes. The product of appropriate swaps yields a reordering operator that is sparse with exactly one entry ± 1 in each row and column. To apply such an operator to either side of $\hat{A} : \mathcal{F}_m \rightarrow \mathcal{F}_n$, requires only $\chi_m \chi_n$ operations, where χ_m and χ_n are the dimensions of the (possibly reduced) incoming and outgoing Hilbert spaces. Every contraction of the operator, except

for partial traces or projections, would however already require a larger number of numerical operations. The computational overhead is hence marginal. There is no overhead in memory requirements.

Further, all considerations about locality, hence, carry over directly from those of the known QUOCs (for instance the qudit MERA) to the corresponding FOC (e.g., the fermionic MERA). In the calculation of local expectation values w.r.t. a MERA, only operators inside a causal cone of the observable enter the actual calculation (all others cancel). That Jordan-Wigner strings outside the causal cone can be avoided for the fermionic MERA has already been shown by an alternative approach in Ref. [239], see also Ref. [240].

8.5. Further operations on FOCs

8.5.1. Hermitian conjugation

The Hermitian conjugate of a FOC is simply given by

$$(\hat{A}_N \circ \dots \circ \hat{A}_1)^\dagger = \hat{A}_1^\dagger \circ \dots \circ \hat{A}_N^\dagger. \quad (8.23)$$

The operator order is reversed and one has to take the Hermitian conjugate of each fermionic operator in the circuit. In the representation as a directed graph, all arcs are reversed. The Hermitian conjugate is, e.g., of interest when calculating expectation values with respect to a (pure) FOC state. Fig. 8.8a shows it for the example of a fermionic PEPS.

8.5.2. Reversing contraction arcs

For algorithms operating on FOCs, as for example the one for fermionic PEPS presented in Sec. 8.6, it is sometimes useful to reverse contraction arcs, i.e., to change outgoing modes of one operator to incoming modes and vice versa at the operators it is contracted with; see Fig. 8.7a. Let $\hat{A} : \mathcal{F}_{m \cup r} \rightarrow \mathcal{F}_{n \cup s \cup p}$ and $\hat{B} : \mathcal{F}_{n \cup s \cup q} \rightarrow \mathcal{F}_{k \cup r}$, i.e., the operators outgoing/incoming supports overlap in the modes n, r and s . Let $\mathfrak{m}, \mathfrak{n}, \mathfrak{r}, \mathfrak{s}, \mathfrak{p}, \mathfrak{q}, \mathfrak{k}$ be orderings for the modes in m, n, r, s, p, q , and k . For reversing the arc corresponding to modes n , i.e., changing the modes n to be incoming (outgoing) at operator $\hat{A}$ ($\hat{B}$), the relations between $\hat{A}$ and $\hat{B}$ and the resulting operators (as depicted in Fig. 8.7a) are

$$\begin{aligned} \mathfrak{k} \oplus \mathfrak{r} \langle \mathbf{kr} | \hat{B} | \mathbf{nsq} \rangle_{\mathfrak{n} \oplus \mathfrak{s} \oplus \mathfrak{q}} &= (-1)^{\bar{n}\bar{q}} \mathfrak{k} \oplus \mathfrak{n} \oplus \mathfrak{r} \langle \mathbf{knr} | \hat{B}' | \mathbf{sq} \rangle_{\mathfrak{s} \oplus \mathfrak{q}}, \\ \mathfrak{n} \oplus \mathfrak{s} \oplus \mathfrak{p} \langle \mathbf{ns p} | \hat{A} | \mathbf{mr} \rangle_{\mathfrak{m} \oplus \mathfrak{r}} &= (-1)^{\bar{n}\bar{p}} \mathfrak{s} \oplus \mathfrak{p} \langle \mathbf{sp} | \hat{A}' | \mathbf{mnr} \rangle_{\mathfrak{m} \oplus \mathfrak{n} \oplus \mathfrak{r}}, \end{aligned}$$

such that $\hat{B} \circ \hat{A} = \hat{B}' \circ \hat{A}'$.

8.5.3. Singular value decomposition and truncation

It is possible to decompose an operator $\hat{A} : \mathcal{F}_{m \cup n} \rightarrow \mathcal{F}_{u \cup v}$ by singular value decomposition with respect to arbitrary splittings of the incoming and outgoing modes. The resulting circuits can be chosen to be of the form $\hat{C} \circ \hat{B}$ or $\hat{C} \circ \hat{\Lambda} \circ \hat{B}$, where $\hat{\Lambda} : \mathcal{F}_z \rightarrow \mathcal{F}_x$ ($|x| = |z|$)

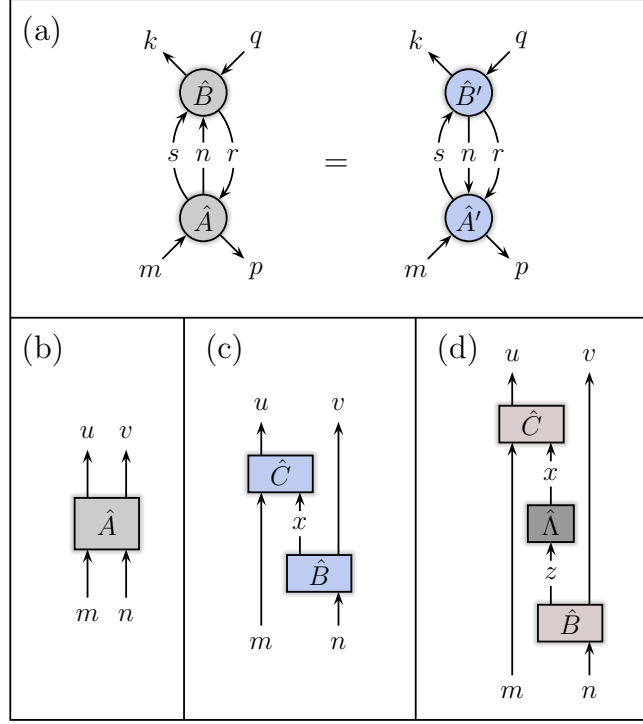


Figure 8.7.: In all subplots, the operator order is defined to increase from the bottom to the top. (a) It is possible to reverse contraction arcs. The resulting operators can be expressed in terms of matrix elements of the original operators; see Sec. 8.5.2. Reversing the arc for modes n yields the sign factor $(-1)^{\bar{n}(\bar{p}+\bar{q})}$. (b–d) It is possible to decompose operators ($\hat{A}$) by singular value decomposition, resulting in circuits of the form (c) or (d). This also allows for the reduction of retained Hilbert space dimensions: Contract operators $\hat{B}$ and $\hat{C}$ to obtain an operator $\hat{A}$, apply the singular value decomposition to it and truncate (some of the smallest) singular values, to obtain an approximation of $\hat{C} \circ \hat{B}$. Reversing contraction arcs and truncation of Hilbert spaces via singular value decomposition are for example employed in the contraction algorithm for fermionic PEPS in Sec. 8.6.

is a diagonal operator encoding the singular values; see Figs. 8.7b–8.7d. This also allows for truncation of modes (or the reduction of Hilbert space dimensions): Contract two operators $\hat{C} : \mathcal{F}_{m \cup x} \rightarrow \mathcal{F}_u$ and $\hat{B} : \mathcal{F}_n \rightarrow \mathcal{F}_{x \cup v}$, as in Fig. 8.7c to obtain an operator $\hat{A}$, apply the singular value decomposition to it and truncate (some of the smallest) singular values, to obtain an approximation of $\hat{C} \circ \hat{B}$ where the dimension of the retained Hilbert space for the modes in x has been reduced.

Let m, n, u, v, x , and z be orderings of modes in m, n, u, v, x , and z . The contraction of the FOC $\hat{C} \circ \hat{B}$, as depicted in Fig. 8.7c yields

$$\begin{aligned} \hat{C} \circ \hat{B} = & (-1)^{\tilde{m}\tilde{v}} |\mathbf{uv}\rangle_{u \oplus v} {}_u \langle \mathbf{u} | \hat{C} | \mathbf{xn} \rangle_{x \oplus n} \\ & \times {}_x \langle \mathbf{xv} | \hat{B} | \mathbf{n} \rangle_n {}_n \langle \mathbf{nm} |. \end{aligned} \quad (8.24)$$

With the occupation number representation $A := J_{u \oplus v, n \oplus m}(\hat{A})$ of $\hat{A}$, one can hence decompose the operator by applying the singular value decomposition to the matrix $\tilde{A}$ defined by

$$(\mathbf{uv} | \tilde{A} | \mathbf{nm}) := (-1)^{\tilde{m}\tilde{v}} (\mathbf{uv} | A | \mathbf{nm}), \quad (8.25)$$

$$\tilde{A} = U \Lambda V, \quad (8.26)$$

where U and V are unitary and Λ is the diagonal matrix of singular values. The operators of the resulting circuit $\hat{C} \circ \hat{B}$ can then be chosen as ($0 < \alpha < 1$)

$$J_{u, x \oplus m}(\hat{C}) = U \Lambda^\alpha, \quad J_{x \oplus v, n}(\hat{B}) = \Lambda^{1-\alpha} V. \quad (8.27)$$

When the singular values are to be separated into a third operator $\hat{\Lambda}$ as depicted in Fig. 8.7d, the operators of the resulting circuit $\hat{C} \circ \hat{\Lambda} \circ \hat{B}$ are given by

$$J_{u, x \oplus m}(\hat{C}) = U, \quad J_{x, z}(\hat{\Lambda}) = \Lambda, \quad J_{z \oplus v, n}(\hat{B}) = V. \quad (8.28)$$

Reduction of Hilbert space dimensions (*truncation*) via singular value decomposition is for example employed in the algorithm for evaluating expectation values with respect to fermionic PEPS in an approximative fashion; see Sec. 8.6.

8.6. Fermionic PEPS

The FOC framework incorporates a fermionic version of the class of qudit states called *tensor product ansätze* [116–118] or *projected entangled pair states* (PEPS) [119]. In Ref. [241] it was suggested to obtain fermionic PEPS by applying fermionic parity-symmetric (projection) operators to a tensor product of maximally entangled pair states. The detour over maximally entangled states is not necessary (but also not harmful); as depicted on the left hand side of Fig. 8.8a, a fermionic PEPS on a square lattice, equivalently, can be defined by assigning to each lattice site (x, y) (away from the boundaries) a parity-symmetric fermionic operator $\hat{A} : \mathcal{F}_{a \cup m} \rightarrow \mathcal{F}_{b \cup n \cup s}$ where a and m are sets of incoming

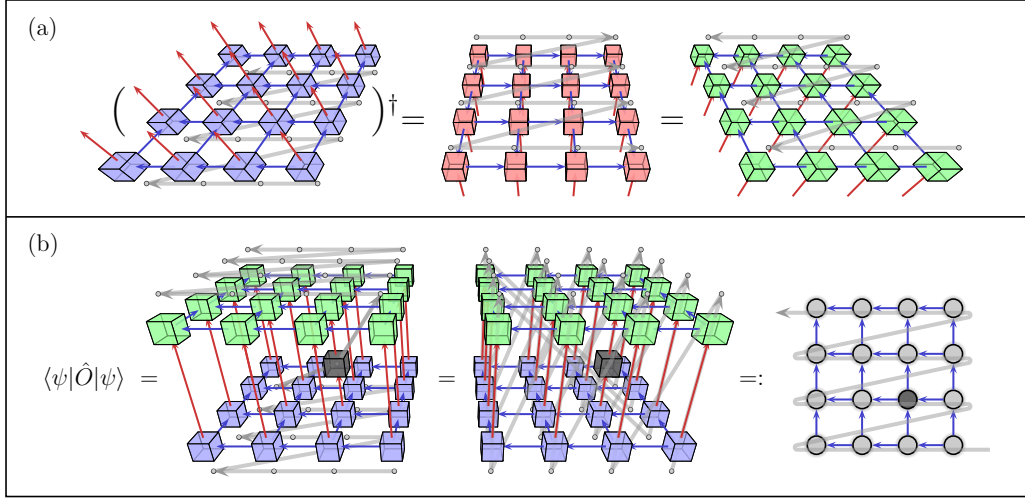


Figure 8.8.: (a) A fermionic PEPS can be constructed as a FOC, where fermionic operators are assigned to each lattice site. As chosen here for a square lattice, each operator has two sets of incoming modes from operators on neighboring sites and two outgoing sets of modes to operators of the remaining nearest neighbors. One outgoing set of modes corresponds to the physical site Hilbert space. The Hermitian conjugate of the circuit $\hat{A}_N \circ \dots \circ \hat{A}_1$ is $\hat{A}_1^\dagger \circ \dots \circ \hat{A}_N^\dagger$. All contraction arcs and the operator order (gray line below/above the circuit) are reversed. This side effect can be reverted (without changing the value of the FOC) by applying Eq. (8.21) and the rule derived in Sec. 8.5.2 with only a marginal computational overhead. (b) To evaluate a local expectation value, the FOCs for bra, local observable, and ket have to be composed. The operator order can again be changed for later convenience – in this case no additional sign factors occur, as all swapped operators have no common contraction arcs. For the definition of the objects on the right hand side, see also Fig. 8.9a.

modes from operators on neighboring sites $(x+1, y)$ and $(x, y+1)$, and b and n are outgoing modes to operators on sites $(x-1, y)$ and $(x, y-1)$. The set of modes s composes the local physical Hilbert space of site (x, y) . In the FOC framework, the generalization to more complicated or higher-dimensional lattices is straightforward. The choice of the direction of the contraction arcs is (an arbitrary) part of the definition of the state and can also be changed later as described in Sec. 8.5.2. To complete the definition of the fermionic PEPS one needs to specify an (initial) operator order. An example is given on the left hand side of Fig. 8.8a, where the gray line below the lattice indicates the lexicographic order with respect to lattice coordinates $(-x, y)$.

In Ref. [241] it was described how the FOC of a fermionic PEPS can be mapped to a QUOC by choosing a fixed ordering of all modes. This was achieved with one additional bond per horizontal contraction arc (i.e., a factor of four in the number of degrees of free-

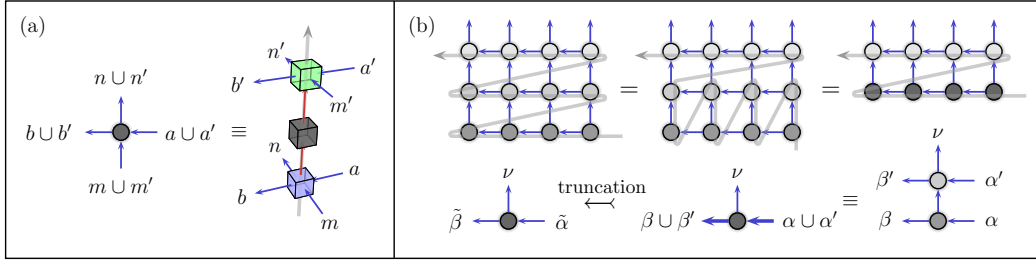


Figure 8.9.: (a) Definition of the objects on the right hand side of Fig. 8.8b – here, in particular, for the site where the local observable acts nontrivially. (b) The FOC for the evaluation of a local observable is contracted by considering the first row of the FOC as a state $|\chi_1\rangle$ and applying the other rows as operators to it $|\chi_y\rangle = \hat{T}_y|\chi_{y-1}\rangle$. Doing this in an exact manner, the number of degrees of freedom per site for the states $|\chi_y\rangle$ would in general increase exponentially with y . One can decrease them during the algorithm for the case of a finite (infinite, translationally invariant) lattice by applying the DMRG (iTEBD) algorithm.

dom per site) and a correspondingly reduced computational efficiency (a factor of several powers of four) for the evaluation of expectation values, calculation of ground states etc.

The approach presented here is an alternative one, emphasizing that the mapping to a QUOC (with a fixed mode order) is not necessary. All manipulations and contractions on fermionic PEPS can be done according to the rules described in Secs. 8.2, 8.3, and 8.5. In that case, compared to the same operations on a corresponding qudit PEPS (replacing the fermionic operators with qudit operators of identical dimensions), only marginal computational overheads arise.

Fig. 8.8 shows graphically how the FOC for the evaluation of a local expectation value $\langle\psi|\hat{O}|\psi\rangle$ can be constructed. For the bra vector (dual vector) $\langle\psi|$, operator order and contraction lines reverse as a side effect of taking the Hermitian conjugate; Sec. 8.5.1. For later convenience this is reverted by applying Eq. (8.21) and the rule derived in Sec. 8.5.2. After composing bra, observable, and ket, the operator order can again be changed conveniently, this time without any sign factors occurring, as all swapped operators share no common contraction arcs; Fig. 8.8b. As in the qudit case [119], the contraction of the resulting circuit can be executed row by row, i.e., by treating the lowest row as a one-dimensional state $|\chi_1\rangle$ to which the operators of the following row $\hat{T}_y$ (row transfer matrix) are applied; $|\chi_y\rangle = \hat{T}_y|\chi_{y-1}\rangle$. No additional sign factors occur due to operator reorderings (Fig. 8.9), but only due to mode reorderings (Sec. 8.2.1) before contractions (marginal overhead). An essential aspect of PEPS algorithms is that contractions, e.g., for the evaluation of expectation values, cannot be executed exactly, as the stepwise application of the row transfer matrices would in general lead to an exponential growth in the number of modes per site for $|\chi_y\rangle$. As suggested in Ref. [119], this can be circumvented by applying a variant of the density-matrix renormalization-group (DMRG) algorithm [66, 68] to each state $|\chi_y\rangle$, be-

fore executing the contractions to the next row. The only purpose of the DMRG procedure is here to reduce the number of degrees of freedom in each step to a manageable number, and hence, do contractions in an approximative fashion. The essential operation is to do Schmidt decompositions of χ_y . This can be done for FOCs as described in Sec. 8.5.3.

The FOC framework also allows to simulate infinite fermionic PEPS. To this purpose, the fermionic PEPS is to be defined by repetition of an elementary cell FOC; see Ref. [126] for the qudit case. The algorithm does not deviate substantially from the finite-size case. The biggest difference being that, for the reduction of degrees of freedom in states χ_y , one has to use a translationally invariant formulation of the DMRG algorithm, basically the iTEBD algorithm as described in Ref. [250], again based on the ability to do singular value decompositions (Sec. 8.5.3). With this, one has a translation of the algorithms for the calculation of approximative ground state or time-evolved qudit (i)PEPS [119, 126] to the fermionic case without reduction of the computational efficiency, as those algorithms are based on the ability to contract operator circuits just as in our example.

8.7. Discussion

In chapter 7 (see also Ref. [239]) it was shown that contractions of fermionic unitary circuits with a causal cone (e.g., the evaluation of local observables w.r.t. a MERA) can be done without occurrence of any Jordan-Wigner strings outside the causal cone. Here, this result was extended in proving that arbitrary parity-symmetric fermionic operator circuits can actually be contracted with the *same* computational effort and memory requirements as a corresponding QUOC. This remarkable result follows from the fact that a given contraction sequence for a QUOC can be implemented for a corresponding FOC with essentially the same number of computational operations. The required contraction primitives have been presented and the marginal computational overheads been discussed.

This allows to translate algorithms on QUOCs to corresponding algorithms on FOCs. For example in the algorithm for scale-invariant MERA as studied in Refs. [129, 251, 252], the super operator simply becomes a fermionic super operator. Its iterative application to an observable yields the expectation value of the observable in the thermodynamic limit.

For the special example of the FOC being a MERA, in Ref. [240], first numerical results were presented (postponing a description of the algorithm for a later publication). A scheme for fermionic PEPS was suggested in Ref. [241]. The suggested mapping to a QUOC used there seems numerically less efficient than the contraction scheme presented here. Instead of encoding the fermionic sign factors by increasing tensor dimensions, they can be taken account of during contractions, specifically in preparative mode reorderings, and operator order swaps. The resulting marginal overhead appears smaller.

It will be interesting to see to what extent variational ansätze like fermionic variants of PEPS or MERA, both satisfying entropic area laws [115, 253], will be able to appropriately grasp the correlations present in critical fermionic strongly correlated models, models that are known to violate such area laws logarithmically [103, 102, 105, 106, 254]. First numerical results [240, 241, 239] seem promising. It is the hope that the framework dis-

cussed in this work will help in constructing fermionic variants of variational approaches to simulate strongly correlated fermions in higher dimensions.

8.8. Alternative derivation of the rule for partial multiplications

For the same preconditions as in Sec. 8.2.2, let us derive the partial multiplication rule – this time by extending the supports of operators $\hat{A}$ and $\hat{B}$ prior to the contraction.

Let $\hat{D} : \mathcal{F}_m \rightarrow \mathcal{F}_n$, and let $\mathfrak{m}, \mathfrak{n}, \mathfrak{r}$ be orderings of the modes in m, n , and r . Extending the incoming and outgoing supports of $\hat{D}$ by modes r (on which the resulting operator is supposed to act trivially), one arrives at $\hat{D}' : \mathcal{F}_{m \cup r} \rightarrow \mathcal{F}_{n \cup r}$ with

$$\hat{D}' = |\mathfrak{n}\mathfrak{r}\rangle_{\mathfrak{n} \oplus \mathfrak{r}} \mathfrak{n} \langle \mathfrak{n} | \hat{D} | \mathfrak{m} \rangle_{\mathfrak{m} \oplus \mathfrak{r}} \langle \mathfrak{m}\mathfrak{r} |. \quad (8.29)$$

This is confirmed by $\text{Tr}_r \hat{D}' = \hat{D}$, according to (8.15), and $\hat{f}_x \hat{D}'_{\pm} = \pm \hat{D}'_{\pm} \hat{f}_x$ for all $x \in r$.

Using the rule (8.29) to extend the supports of the operators $\hat{A} : \mathcal{F}_m \rightarrow \mathcal{F}_{n \cup p}$ and $\hat{B} : \mathcal{F}_{n \cup q} \rightarrow \mathcal{F}_k$ by modes q and p , respectively, defines operators $\hat{A}' : \mathcal{F}_{m \cup q} \rightarrow \mathcal{F}_{n \cup p \cup q}$ and $\hat{B}' : \mathcal{F}_{n \cup p \cup q} \rightarrow \mathcal{F}_{k \cup p}$. The partial multiplication $\hat{C} = \hat{B} \cdot_n \hat{A}$ amounts now simply to the usual operator product $\hat{C} = \hat{B}' \cdot \hat{A}'$. Assuming we have the two operators in representations $A = J_{\mathfrak{a}, \mathfrak{m}}(\hat{A})$ and $B = J_{\mathfrak{k}, \mathfrak{b}}(\hat{B})$ with $\mathfrak{a} = \mathfrak{n} \oplus \mathfrak{p}$ and $\mathfrak{b} = \mathfrak{n} \oplus \mathfrak{q}$ ($\mathfrak{p}$ and $\mathfrak{q}$ are orderings for the modes in p , and q),

$$\hat{A}' = |\mathfrak{n}\mathfrak{p}\mathfrak{q}\rangle_{\mathfrak{a} \oplus \mathfrak{q}} \mathfrak{a} \langle \mathfrak{n}\mathfrak{p} | \hat{A} | \mathfrak{m} \rangle_{\mathfrak{m} \oplus \mathfrak{q}} \langle \mathfrak{m}\mathfrak{q} |,$$

and

$$\begin{aligned} \hat{B}' &= |\mathfrak{k}\mathfrak{p}\rangle_{\mathfrak{k} \oplus \mathfrak{p}} \mathfrak{k} \langle \mathfrak{k} | \hat{B} | \mathfrak{n}\mathfrak{q} \rangle_{\mathfrak{b} \oplus \mathfrak{p}} \langle \mathfrak{n}\mathfrak{q}\mathfrak{p} | \\ &= (-1)^{\bar{p}\bar{q}} |\mathfrak{k}\mathfrak{p}\rangle_{\mathfrak{k} \oplus \mathfrak{p}} (\mathfrak{k} | B | \mathfrak{n}\mathfrak{q})_{\mathfrak{n} \oplus \mathfrak{p} \oplus \mathfrak{q}} \langle \mathfrak{n}\mathfrak{p}\mathfrak{q} |. \end{aligned}$$

The result $\hat{C} : \mathcal{F}_{m \cup q} \rightarrow \mathcal{F}_{k \cup p}$ of the multiplication with orderings $\mathfrak{c}_1 = \mathfrak{k} \oplus \mathfrak{p}$, $\mathfrak{c}_2 = \mathfrak{m} \oplus \mathfrak{q}$ is then

$$\begin{aligned} \hat{C} &= \hat{B}' \cdot \hat{A}' \\ &= (-1)^{\bar{p}\bar{q}} |\mathfrak{k}\mathfrak{p}\rangle_{\mathfrak{k} \oplus \mathfrak{p}} (\mathfrak{k} | B | \mathfrak{n}\mathfrak{q}) (\mathfrak{n}\mathfrak{p} | A | \mathfrak{m})_{\mathfrak{m} \oplus \mathfrak{q}} \langle \mathfrak{m}\mathfrak{q} | \\ &= |\mathfrak{k}\mathfrak{p}\rangle_{\mathfrak{c}_1} (\mathfrak{k}\mathfrak{p} | C | \mathfrak{m}\mathfrak{q})_{\mathfrak{c}_2} \langle \mathfrak{m}\mathfrak{q} |, \end{aligned}$$

coinciding with Eq. (8.10).

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Publication list

During the course of the work for this thesis several articles have been published or made available as preprints on arxiv.org. The content of papers on the *scaling and evolution of entanglement entropy* in many-particle systems

- H.-Q. Zhou, T. Barthel, J. O. Fjærestad, and U. Schollwöck: *Entanglement and boundary critical phenomena*, Phys. Rev. A **74**, 050305(R) (2005),
- T. Barthel, M.-C. Chung, and U. Schollwöck: *Entanglement scaling in critical two-dimensional fermionic and bosonic systems*, Phys. Rev. A **74**, 022329 (2006),
- T. Barthel, S. Dusuel, and J. Vidal: *Entanglement entropy beyond the free case*, Phys. Rev. Lett. **97**, 220402 (2006),
- J. Vidal, S. Dusuel, and T. Barthel: *Entanglement entropy in collective models*, J. Stat. Mech. P01015 (2006),
- T. Barthel and U. Schollwöck: *Dephasing and the steady state in quantum many-particle systems*, Phys. Rev. Lett. **100**, 100601 (2008),

and of those on *simulation methods* of such systems via classes of *ansatz states*

- T. Barthel, U. Schollwöck, and S. R. White: *Spectral functions in one-dimensional quantum systems at finite temperature using the density matrix renormalization group*, Phys. Rev. B **79**, 245101 (2009),
- C. Pineda, T. Barthel, and J. Eisert: *Unitary circuits for strongly correlated fermions*, arXiv:0905.0669 (2009),
- T. Barthel, C. Pineda, and J. Eisert: *Contraction of fermionic operator circuits and the simulation of strongly correlated fermions*, Phys. Rev. A **80**, 042333 (2009),

partially entered the thesis.

Two further publications are more experimentally motivated and concern specific effects and suggestions for experiments for *ultracold atomic gases in optical lattices* [255]:

- G. Roux, T. Barthel, I. P. McCulloch, C. Kollath, U. Schollwöck, and T. Giamarchi: *Quasiperiodic Bose-Hubbard model and localization in one-dimensional cold atomic gases*, Phys. Rev. A **78**, 023628 (2008).
- T. Barthel, C. Kasztelan, I. P. McCulloch, and U. Schollwöck: *Magnetism, coherent many-particle dynamics, and relaxation with ultracold bosons in optical superlattices*, Phys. Rev. A **79**, 053627 (2009).

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