Entanglement and its facets in condensed matter systems

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Erklärung

Die vorliegende Habilitationsschrift gibt eine Übersicht über Forschungsergebnisse, welche bereits - bis auf Paragraph 4.3 - in wissenschaftlichen Zeitschriften veröffentlicht wurden. Die relevanten Publikationen dazu sind

- A. Osterloh, L. Amico, G. Falci, and R. Fazio, *Scaling of the Entanglement close to Quantum Phase Transitions*, Nature **416**, 608-610 (2002).
- L. Amico and A. Osterloh, *Out of equilibrium correlation functions of quantum anisotropic XY models: one-particle excitations*, J.Phys. A **37**, 291 (2004).
- L. Amico, A. Osterloh, F. Plastina, R. Fazio, and M. Palma, *Dynamics of Entanglement in One-Dimensional Spin Systems*, Phys. Rev. A. **69**, 022304 (2004). Selected for publication in the February issue of the Virtual Journal of Nanoscale Science & Technology, 2004 and in the February issue of the Virtual Journal of Quantum Information, 2004.
- F. Plastina, L. Amico, A. Osterloh, and R. Fazio, *Spin wave contribution to entanglement in Heisenberg models*, New J. Phys. **6**, 124 (2004).
- L. Amico, A. Osterloh, F. Plastina, and R. Fazio, *Entanglement in One-Dimensional Spin Systems*, to appear in the Proceedings of the SPIE defense and security, Orlando, Florida, USA (2004).
- A. Osterloh, J. Siewert, *Constructing N-qubit entanglement monotones from anti-linear operators*, Phys. Rev. A **72**, 012337 (2005). Selected for publication in the August 2005 issue of the Virtual Journal of Quantum Information
- A. Osterloh and J. Siewert, *Entanglement monotones and maximally entangled states for multipartite qubit systems*, Int. J. Quant. Inf. **4**, 531 (2006).
- R. Lohmeyer, A. Osterloh, J. Siewert, and A. Uhlmann, *Entangled three-qubit states without concurrence and three-tangle*, Phys. Rev. Lett **97**, 260502 (2006).
- A. Osterloh, G. Palacios, and S. Montangero *Enhancement of pairwise entanglement from $\mathbb{Z}_2$ symmetry breaking*, Phys. Rev. Lett **97**, 257201 (2006). Selected for the July 3, 2007 issue of the Virtual Journal of Nanoscale Science & Technology.
- L. Amico, R. Fazio, A. Osterloh, and V. Vedral, review on *Entanglement in Many-Body Systems*, quant-ph/0703044 submitted to Review of Modern Physics.

Ich erkläre hiermit, daß alle zur Ausführung der vorliegenden Arbeit benötigten Hilfsmittel und Referenzen zitiert werden.

Andreas Osterloh
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\[1\text{Jede der so vielen praktisch unwiderstehlichen Pasticceri siciliane wurde dabei mit eingerechnet!}\]
Die Anwesenheit verschränkter Quantenzustände führte zu Unbehagen und Zweifeln an der Quantentheorie, ob der Nichtlokalität, die sie in sich tragen. Da Lokalität einer der Hauptpfeiler physikalischer Gedankengebäude war und noch ist, wurde die Annahme der Unvollständigkeit der Quantentheorie und damit die Existenz versteckter lokaler Variablen geboren. Es war die bahnbrechende Arbeit von John Bell, die es möglich machte, anhand von sogenannten „Bellungleichungen“ die Vorhersagen der Quantentheorie von denen einer Theorie mit versteckten Variablen zu unterscheiden; bislang sind derartige Messungen zugunsten der Quantentheorie ausgefallen. Es ist seit der Gründung der Quanteninformationstheorie, daß die Verschränktheit von Zuständen - das „Entanglement“ - wieder in den Mittelpunkt des Interesses gerückt ist, und zwar als Ressource für die Ausführung klassisch unmöglicher Prozesse, wie etwa der Teleportation. Dieser Aspekt führte unausweichlich zu dem Bestreben wissenschaftlicher Arbeiten, diese Ressource klassifizieren und natürlich auch quantifizieren zu wollen. Zu diesem Zwecke sind Minimalkriterien an ein Maß für Entanglement erarbeitet worden, welche auf das Konzept des „Entanglement Monotones“ führten. Dieses Fundament motivierte nachfolgend lebhafte wissenschaftliche Aktivität mit Fokus auf das Entanglement von Bipartitionen, welche wichtige Kriterien wie den Schmidt-Rang, die von Neumann Entropie und die „Concurrence“ hervorbrachten. Der Erfolg bei bipartiten Systemen rief nach Erweiterungen der dort gefundenen Resultate auf multipartite Systeme; jedoch erwies sich dieses neue Feld als weitaus komplizierter. Ausschlaggebend hierfür ist letztlich die parallele Existenz verschiedener Entanglementsklassen bezüglich stochastisch lokaler Transformationen begleitet von klassischer Kommunikation (SLOCC).

Von vor etwa zehn Jahren entstammte die Idee, daß die Quanteninformationstheorie das Potential haben könnte, ein tieferes Verständnis von komplexen Phänomenen im Bereich der kondensierten Materie oder der Quantenfeldtheorie zu erlangen. Tatsächlich führte die darauffolgende intensive Forschungsarbeit unter dieser Prämissen auf beiden Gebieten zu einer wechselseitigen Befruchtung. Von der dramatisch anwachsenden Intensität wissenschaftlicher Arbeit auf dem Überlapp beider Gebiete profitierten beide Seiten. Als besonders relevant für die vorliegende Arbeit sei hier die Untersuchung von Entanglementaspekten in der Nähe quantenkritischer Punkte zu nennen; jedoch führte die Sichtweise der Quanteninformationstheorie auch schon zu wichtigen Modifikationen numerischer Simulationsmethoden im Bereiche der kondensierten Materie, wie beispielsweise der DMRG. Desweiteren ist der vielereits erströmte Quantenrechner letztendlich ein großes System von Quanteninformationseinheiten (z.B. Qubits), für welche lokale Operationen, aber auch paarweise Wechselwirkungen untereinander auf kontrollierte Weise manipuliert werden können müssen. Daher sind z.B. Spinketten als Quantenregister, also als Träger von Quanteninformation, bzw. als Quantenkanal vorgeschlagen worden. Im letzteren Falle würde die natürlich gegebene hamilton’sche Zeitentwicklung zum Transport von Quantenbits ausgenutzt werden wollen.

Viele Arbeiten untersuchten also die Dynamik von Entanglement in Systemen kondensierter Materie z.B. unter dem Aspekt optimaler Datenübertragung, oder aber des Entanglementgehalts von Grundzuständen quantenkritischer Mo-
delle. Ein wichtiges und praktisch einhelliges Resultat der Untersuchungen der letzteren Kategorie ist, daß das für Quantenphasenumzüge wichtige Entangle-
glement vornehmlich multipartiter Natur ist. Diese Erkenntnis entfesselt eine Plethora ungelöster Probleme, welche bis in Bereiche der Invariantentheorie rei-
chen. Ohne klare Vorstellung, welche Entanglementsklasse für bestimmte komple-
xe Phänomene von Wichtigkeit sein könnte, wird ein möglicher Zusammenhang
nur schwer hergestellt werden können; aber dafür wäre eine bekannte Klas-
sifizierung des Entanglements Voraussetzung. Dieses Manko führt dazu, daß
zunächst leicht berechenbare Größen analysiert werden, welche aber dennoch
gewisse Schlüsse über das Entanglement im betrachteten System zulassen. Die-
se erzwungen pragmatische Herangehensweise ist zwar wichtig; sie läßt jedoch
viele Facetten des Problems aus, und dürfte daher auf lange Sicht unzureichend
sein.

Die vorliegende Arbeit ist eine Zusammenfassung der in der vorhergehen-
der Erklärung enthaltenen Liste von Publikationen. Nach einer Einführung in
die meistgenutzten Entanglementmaße, greift sie an das Problem des mutmaß-
lichen Zusammenhanges zwischen Entanglement und Quantenphasenumzügen
an und zitiert eine Reihe von Arbeiten zu diesem Thema als Beleg für die Rele-
vanz multipartiter Entanglements. Darauffolgend wird das Problem der Quan-
tifizierung und Klassifizierung „genuin multipartiten Entanglements“ formuliert
und angegangen. Die Schlüsselerkenntnis hierzu ist, die \( SL(2, \mathbb{C}) \) samt Qubitper-
mutationen als Invarianzgruppe zu identifizieren. Lokale antilineare Operatoren
mit verschwindenden Erwartungswerten auf dem gesamten lokalen Hilbertraum
werden als Bausteine für solche Maße vorgestellt. Auf diese Weise konnte ei-
ne vollständige Klassifizierung vierpartiten Entanglements erfolgen, aber auch
Maße für echt multipartites Entanglement für eine beliebige Anzahl von Qubits
sind in Reichweite. Die konstruierten Maße sind zunächst nur wohldefiniert auf
reinen Zuständen; die Erweiterung auf gemischte Zustände mittels des sogenann-
ten „convex roof“ stellt eines der ungelösten Probleme dar. Auf dem Wege zu
dessen Lösung konnten Gemische zweier bestimmter tripartiter Zustände analy-
tisch behandelt werden; einige der Ergebnisse dieser Arbeit lassen sich sogar auf
beliebige Rang-zwei Gemische und für beliebige Anzahl der Qubits übertragen.

Die Konstruktion mit lokalen invarianten Operatoren ist vom physikalischen
Standpunkt besonders sinnvoll, da sie den Grundstein dafür legt, die Entangle-
glementmaße durch Korrelationsfunktionen auszudrücken. Dazu konnte eine eins-
zu-eins-Beziehung von Erwartungswerten antilinearer hermitescher Operato-
ren mit Erwartungswerten eindeutig zugeordneter linearer hermitescher Operato-
ren hergestellt werden. Abschätzungen für das convex roof schwach gemischter
Zustände werden dann eine direkte Anknüpfung an das Experiment liefern.
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Entanglement has been always considered as the counter intuitive part and “spooky” non-locality inherent to quantum mechanics \[15\]. It apparently contradicts one of the basic pillars of physics - locality - and gave rise to severe skepticism for several decades. It was after the seminal contribution of John Bell that the fundamental questions related to the existence of entangled states could be tested experimentally. Under fairly general assumptions, Bell derived a set of inequalities for correlated measurements of two physical observables that any local theory should obey. The overwhelming majority of experiments done so far are in favor of quantum mechanics thus demonstrating that quantum entanglement is physical reality \[97\].

Entanglement has gained renewed interest with the development of quantum information science \[86\]. In its framework, quantum entanglement is viewed at as a precious resource for quantum information processing. It is e.g. believed to be the main ingredient to the quantum speed-up in quantum computation and communication. Moreover several quantum protocols, as teleportation \[18\], can be realized exclusively with the help of entangled states.

The role of entanglement as a resource in quantum information has stimulated intensive research that tries to unveil both its qualitative and quantitative aspects \[24, 16, 41, 146, 100, 101\]. Many criteria have been proposed to distinguish whether a pure state is entangled or not, as for example the Schmidt rank and the von Neumann entropy, and necessary requirements to be satisfied by an entanglement measure have been elaborated and have lead to the notion of an entanglement monotone \[133\]. Since then, a substantial bulk of work appeared on entanglement monotones for bipartite systems, in particular for the case of qubits. The success in the bipartite case for qubits asked for extensions to the multipartite case, but the situation proved to be far more complicated: different classes of entanglement occur, which are inequivalent not only under deterministic local operations and classical communication (LOCC), but even under their stochastic analogue (SLOCC) \[20\].

During the last decade it has been suggested that quantum information science might bear the potential to give further insight into areas of physics as condensed matter or quantum field theory \[104\]. Indeed has the growing interest of the quantum information community in systems from condensed matter

\[1\] There are states that do not violate Bell inequalities and nevertheless are entangled \[81\].
stimulated an exciting cross-fertilization between the two areas; the amount of work at the interface between condensed matter physics and quantum information theory has grown tremendously during the last few years, shining light on many different aspects of both subjects. Methods developed in quantum information have proved to be useful also in the analysis of many-body systems. At the same time, the experience built up over the years in condensed matter physics is valuable for finding new protocols for quantum computation and communication: at the end, a quantum computer will be a many-body system where, differently from the ‘traditional’ situation, the Hamiltonian must be manipulated in a controlled manner. Spin networks have been proposed as quantum channels [21] where the collective dynamics of their low lying excitations is exploited for transporting quantum information. But tools from quantum information theory also start influencing numerical methods as the density matrix renormalization group and the design of new efficient simulation strategies for many-body systems (see for example [134, 135, 132]). Of particular interest for this thesis will be the extensive analysis of entanglement in quantum critical models [90, 88, 137].

One important conclusion from the enormous bulk of work concerned with entanglement at quantum phase transitions is that multipartite quantum correlations are typically playing a dominant role [4]. This establishes an interconnection with the field of invariant theory, where the quantification and classification of multipartite entanglement provides with a plethora of open problems also interesting in mathematics. Without a clear perspective of which multipartite quantum correlations might have relevance for certain complex phenomena in condensed matter physics and - most importantly - in absence of a full classification of entanglement, essentially those measures are investigated that can be easily computed. Though important in its own right, this pragmatic approach waives the main scope behind such an analysis, namely the understanding of the underlying entanglement pattern and its interconnection with complex physical phenomena.

Most of this thesis represents a summary of a selection of work published during the last few years [90, 6, 5, 91, 93, 94, 92, 75, 4]. It will start with an overview over largely employed entanglement measures followed by a selection of results of their analysis for condensed matter systems emphasizing the relevance of multipartite entanglement. Thereafter, the concept of genuine multipartite entanglement is introduced and an approach for the construction of genuine multipartite entanglement measures is presented. Relevant new features appearing in the multipartite case, as compared to bipartite measures, are highlighted, together with an outline of how to measure multipartite entanglement in pure states in the laboratory.
Kapitel 2

Pairwise and Bipartite Entanglement

The problem of measuring entanglement is a vast and lively field of research in its own. Numerous different methods have been proposed for its quantification. In this Section we do not attempt to give an exhaustive review of the field. Rather do we want to introduce those measures that are largely being used to quantify entanglement in many-body systems. Comprehensive overviews of entanglement measures can be found in [24, 16, 146, 100, 101, 63]. Also a method for detecting entanglement is outlined that is based on entanglement witnesses.

2.1 Bipartite entanglement in pure states

Bipartite entanglement of pure states is conceptually well understood, although quantifying it for local dimensions higher than two still bears theoretical challenges [139, 63]. A pure bipartite state is not entangled if and only if it can be written as a tensor product of pure states of the parts. It is an important fact with this respect that for every pure bipartite state $|\psi_{AB}\rangle$ (with the two parts, $A$ and $B$), two orthonormal bases $\{ |\psi_{A,i}\rangle \}$ and $\{ |\phi_{B,j}\rangle \}$ exist such that $|\psi_{AB}\rangle$ can be written as

$$|\psi_{AB}\rangle = \sum_i \alpha_i |\psi_{A,i}\rangle |\phi_{B,i}\rangle \quad (2.1)$$

where $\alpha_i$ are positive coefficients. This decomposition is called the Schmidt decomposition and the particular basis coincide with the eigenbasis of the corresponding reduced density operators

$$\rho_B = \text{tr}_A( |\psi_{AB}\rangle \langle \psi_{AB}| ) = \sum_i \alpha_i^2 |\psi_{B,i}\rangle \langle \psi_{B,i}| ,$$

$$\rho_A = \text{tr}_B( |\psi_{AB}\rangle \langle \psi_{AB}| ) = \sum_i \alpha_i^2 |\phi_{A,i}\rangle \langle \phi_{A,i}| .$$

The density operators $\rho_A$ and $\rho_B$ have common spectrum, in particular are they equally mixed. Since only product states lead to pure reduced density matrices, a measure for their mixedness points a way towards quantifying entanglement in
this case. Given the state $|\psi_{AB}\rangle$, we can thus take its Schmidt decomposition, Eq. (2.1), and use a suitable function of the $\alpha_i$ to quantify the entanglement.

It is interesting that an entanglement measure $E$ is fixed uniquely after imposing the following conditions

1. $E$ is invariant under local unitary operations ($\Rightarrow E$ is indeed a function of the $\alpha_i$’s only).
2. $E$ is continuous (in a certain sense also in the asymptotic limit of infinite copies of the state; see e.g. Ref. [101]).
3. $E$ is additive, when several copies of the system are present:
$$E(|\psi_{AB}\rangle \otimes |\phi_{AB}\rangle) = E(|\psi_{AB}\rangle) + E(|\phi_{AB}\rangle).$$

The unique measure of entanglement satisfying all the above conditions is the von Neumann entropy of the reduced density matrices

$$S(\rho_A) = S(\rho_B) = -\sum_i \alpha_i^2 \log(\alpha_i^2),$$  \hspace{1cm} (2.2)\)

this is just the Shannon entropy of the moduli squared of the Schmidt coefficients. In other words: one possible answer on the question of how entangled a bipartite pure state is, can be given by the von Neumann entropy of (either of) the reduced density matrices. The amount of entanglement is generally difficult to define once we are away from bipartite states, but in several cases we can still gain some insight into many-party entanglement if one considers different bipartitions of a multipartite system. In particular if no reduced density matrix is pure, then the state is called globally entangled.

It is worth to notice that a variety of purity measures are admissible when the third condition on additivity is omitted. In principle, there are infinitely many measures for the mixedness of a density matrix; two of them will typically lead to a different ordering when the Hilbert space of the parts has a dimension larger than two. This is essentially equivalent to saying that different inequivalent classes of entanglement exist in these cases. In contrast, if we trace out one of two qubits the corresponding reduced density matrix $\rho_A$ contains only a single independent and unitarily invariant parameter: its smallest eigenvalue. This implies that each monotonic function $[0, 1/2] \mapsto [0, 1]$ of this eigenvalue can be used as an entanglement measure. Though, also here an infinity of different mixedness measures exists, here all lead to the same ordering of states with respect to their entanglement, and in this sense all are equivalent. A relevant example is the (one-) tangle \[30\]

$$\tau_1[\rho_A] := 4\det\rho_A.$$  \hspace{1cm} (2.3)\)

By expressing $\rho_A$ in terms of spin form factors

$$\rho_A = \begin{pmatrix} \frac{1}{2} + \langle S^z \rangle & \langle S^x \rangle - i \langle S^y \rangle \\ \langle S^x \rangle + i \langle S^y \rangle & \frac{1}{2} - \langle S^z \rangle \end{pmatrix},$$  \hspace{1cm} (2.4)\)

where $\langle S^\alpha \rangle = tr_B(\rho_A S^\alpha)$ and $S^\alpha = \frac{1}{2} \sigma^\alpha$, $\sigma^\alpha$ \{\(\alpha = x, y, z\)\} being the Pauli matrices, it follows that

$$\tau_1[\rho_A] = 1 - 4(\langle S^x \rangle^2 + \langle S^y \rangle^2 + \langle S^z \rangle^2).$$

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For a pure state $|\psi_{AB}\rangle$ of two qubits the relation

$$\tau_1 \equiv |\langle \psi^* | \sigma^1_A \otimes \sigma^1_B | \psi \rangle|^2 =: C |\psi_{AB}\rangle|^2 =: \tau_2 \quad (2.5)$$

applies, where $C$ is called the pure state concurrence [59,145], and $*$ indicates the complex conjugation in the eigenbasis of $\sigma^z$. It is worth emphasizing already here that all measures of pairwise qubit entanglement can hence be expressed in terms of the modulus squared of the expectation value of an antilinear operator. This innocent looking detail enhances the minimally required invariance with respect to local $SU(2)$ transformations to the local invariance group $SL(2)$. The latter is known to be the relevant invariance group for the classification of entanglement into SLOCC classes, where generalized local measurements are admitted in a probabilistic way [38]. This observation will be a key element, paving the way towards the quantification and classification of multipartite entanglement.

The von Neumann entropy can be expressed as a function of the (one-) tangle

$$S[\rho_A] = h \left( \frac{1}{2} \left( 1 + \sqrt{1 - \tau_1[\rho_A]} \right) \right)$$

where $h(x) =: -x \log_2 x - (1-x) \log_2 (1-x)$ is the binary entropy. Both the tangle and the concurrence lead to the important monogamy inequality [30,89] which will be discussed in the next Section.

### 2.2 Pairwise qubit entanglement in mixed states

Subsystems of a many-body (pure) state will generally be in a mixed state, and then even different concepts of entanglement do exist. Three important representatives are the entanglement cost $E_C$, the distillable entanglement $E_D$ (both defined in Ref. [17]) and the entanglement of formation $E_F$ [19]. Whereas $E_D$ and $E_C$ are asymptotic limits of multi-copy extraction probabilities of Bell states and creation from such states, the entanglement of formation is the amount of pure state entanglement needed to create a single copy of the mixed state. Very recently, a proof of the full additivity of $E_F$ has been presented [96], which implies that for bipartite systems both concepts coincide (see e.g. [136]), i.e. $E_D = E_C$. The conceptual difficulty behind the calculation of $E_F$ lies in the infinite number of possible decompositions of a density matrix. Therefore, even knowing how to quantify bipartite entanglement in pure states, we cannot simply apply this knowledge to mixed states in terms of an average over the mixtures of pure state entanglement. The problem is that two decompositions of the same density matrix usually lead to a different average entanglement. Which one do we choose? It turns out that we must take the minimum over all possible decompositions, simply because if there is a decomposition where the average is zero, then this state can be created locally without need of any entangled pure state, and therefore $E_F = 0$. The same conclusion can be drawn from the requirement that entanglement must not increase on average by means of local operations including classical communication (LOCC). A minimal set of requirements every entanglement measure has to fulfill has lead to the notion of an entanglement monotone [133].

The entanglement of formation of a state $\rho$ is therefore defined as

$$E_F(\rho) := \min \sum_j p_j S(\rho_{A,j}) \, , \quad (2.6)$$
where the minimum is taken over all realizations of the state $\rho_{AB} = \sum_j p_j |\psi_j\rangle \langle \psi_j|$, and $S(\rho_{A,j})$ is the von Neumann entropy of the reduced density matrix $\rho_{A,j} := \text{tr}_B |\psi_j\rangle \langle \psi_j|$. Eq. (2.6) is the so-called convex roof of the entanglement of formation for pure states, and a decomposition leading to this convex roof value is called an optimal decomposition.

For systems of two qubits, an analytic expression for $E_F$ does exist and it is given by

$$E_F(\rho) = -\sum_{\sigma = \pm} \sqrt{1 + \sigma C^2(\rho)} \ln \frac{\sqrt{1 + \sigma C^2(\rho)}}{2}$$

(2.7)

where $C(\rho)$ is the convex roof of the pure state concurrence [145, 146] which has been defined in the previous section. Its convex roof extension is encoded in the positive Hermitean matrix

$$R \equiv \sqrt{\rho} \rho \sqrt{\rho} = \sqrt{\rho(\sigma^y \otimes \sigma^y)\rho^*(\sigma^y \otimes \sigma^y)} \sqrt{\rho},$$

(2.8)

with eigenvalues $\lambda_1^2 \geq \cdots \geq \lambda_4^2$ in the following way:

$$C = \max\{\lambda_1 - \lambda_2 - \lambda_3 - \lambda_4, 0\}. \quad (2.9)$$

As the entanglement of formation is a monotonous function of the concurrence, also $C$ itself or its square $\tau_2$ can be used as entanglement measures. This is possible due to a curious peculiarity of two-qubit systems: namely that a continuous variety of optimal decompositions exist [145]. The concurrence $C$ and the tangle $\tau$ both range from 0 (no entanglement) to 1.

By virtue of (2.8) and (2.9), the concurrence in a spin-1/2 chain can be computed in terms of up to two-point spin correlation functions. For simplicity we consider a case where the model has a parity symmetry. For this case the reduced density matrix $\rho_{ij}$ for spins placed at sites $i$ and $j$ assumes a simple form in the basis $\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$:

$$\rho_{ij}^{(2)} = \begin{pmatrix} a_{ij} & 0 & c_{ij} \\ 0 & x_{ij} & z_{ij} \\ c_{ij}^* & 0 & b_{ij} \end{pmatrix}, \quad (2.10)$$

with real $a, b, x, y$, and complex $c, z$. The concurrence results to be

$$C_{ij} = 2 \max\{0, |c_{ij}| - \sqrt{x_{ij}y_{ij}}, |z_{ij}| - \sqrt{a_{ij}b_{ij}}\}. \quad (2.11)$$

For translational invariant systems: $x = y$; for real Hamiltonians and stationary states: $c, z \in \mathbb{R}$. Each entry of the matrix $\rho_{ij}$ is then simply related to one- and two-point correlation functions,

$$C_{ij} = 2 \max\{0, C_{ij}^I, C_{ij}^{II}\}. \quad (2.12)$$

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1. $\tilde{\rho} := (\sigma^y \otimes \sigma^y)\rho^*(\sigma^y \otimes \sigma^y)$ is the tilde-conjugate of the density matrix, which here coincides with its time reversal.

2. In this case all the components of the wave function have an even (or odd) number of flipped spins.

3. When discussing qubits or spin-1/2 systems both notations $|0\rangle, |1\rangle$ and $|\uparrow\rangle, |\downarrow\rangle$ will be used for the eigenstates of $S^z$. 

16
where

\[ C^I_{ij} = |g^{xx}_{ij} + g^{yy}_{ij}| - \sqrt{\left(\frac{1}{4} + g^{zz}_{ij}\right)^2 - M_z^2}, \] (2.13)

\[ C^{II}_{ij} = |g^{xx}_{ij} - g^{yy}_{ij}| + g^{zz}_{ij} - \frac{1}{4}, \] (2.14)

with \( g^{\alpha\alpha}_{ij} = \langle S_\alpha^i S_\alpha^j \rangle \) and \( M_z = \langle S_z \rangle \) (assuming translational invariance). A state with dominant fidelity of parallel and anti-parallel Bell states is characterized by dominant \( C^I \) and \( C^{II} \), respectively. This was shown in [46], where the concurrence was expressed in terms of the fully entangled fraction as defined in [110].

The importance of the tangle and the concurrence is due to the monogamy inequality derived in [30] for three qubits. This inequality has been proved to hold also for n-qubits system [89]. In the case of many-qubits (the tangle may depend on the site \( i \)) it reads

\[ \sum_{j \neq i} C^2_{ij} \leq \tau_{1,i}. \] (2.15)

The so called residual tangle \( \tau_{1,i} = \sum_{j \neq i} C^2_{ij} \) is then a measure for multipartite entanglement [30] [89] not stored in pairs of qubits only. We finally mention that the antilinear form of the concurrence was the key for the first explicit construction of a convex roof, and hence its extension to mixed states [59, 145, 123].

Another measure of entanglement we mention is the relative entropy of entanglement [127]. It can be applied to any number of qubits in principle (or any dimension of the local Hilbert space). It is formally defined as \( E(\sigma) := \min_{\rho \in D} S(\sigma||\rho) \), where \( S(\sigma||\rho) = \text{tr} \sigma [\ln \sigma - \ln \rho] \) is the quantum relative entropy. This relative entropy of entanglement quantifies the entanglement in \( \sigma \) by its distance from the set \( D \) of separable states. The main difficulty in computing this measure is to find the disentangled state closest to \( \rho \). This is in general a difficult task, even for two qubits. In the presence of certain symmetries - which is the case for e.g. eigenstates of certain models - an analytical access is possible. In these cases, the relative entropy of entanglement becomes a very useful tool. The relative entropy reduces to the entanglement entropy in the case of pure bipartite states; this also means that its convex roof extension coincides with the entanglement of formation, and is readily deduced from the concurrence [145].

2.3 Localizable entanglement

A different approach to entanglement in many-body systems arises from the quest to swap or transmute different types of multipartite entanglement into pairwise entanglement between two parties by means of generalized measures on the rest of the system. In a system of interacting spins on a lattice one could then try to maximize the entanglement between two spins (at positions \( i \) and \( j \)) by performing measurements on all the others. The system is then partitioned in three regions: the sites \( i, j \) and the rest of the lattice. This concentrated pairwise entanglement can then be used e.g. for quantum information processing. A standard example is that the three qubit GHZ state \( (1/\sqrt{2})(|000\rangle + |111\rangle) \)
after a projective measure in \(x\)-direction on one of the sites is transformed into a two qubit Bell state.

The concept of localizable entanglement has been introduced in [131, 103]. It is defined as the maximal amount of entanglement that can be localized, on average, by doing local measurements in the rest of the system. In the case of \(N\) parties, the possible outcomes of the measurements on the remaining \(N - 2\) particles are pure states \(\ket{\psi_s}\) with corresponding probabilities \(p_s\). The localizable entanglement \(E_{\text{loc}}\) on the sites \(i\) and \(j\) is defined as the maximum of the average entanglement over all possible outcome states \(\ket{\psi_s}_{ij}\)

\[
E_{\text{loc}}(i, j) = \sup_{\mathcal{E}} \sum_s p_s E(\ket{\psi_s}_{ij})
\]  

(2.16)

where \(\mathcal{E}\) is the set of all possible outcomes \((p_s, \ket{\psi_s})\) of the measurements, and \(E\) is the chosen measure of entanglement of a pure state of two qubits (e.g. the concurrence). Although very difficult to compute, lower and upper bounds have been found which allow to deduce a number of consequences for this quantity.

An upper bound to the localizable entanglement is given by the entanglement of assistance [68] obtained from localizable entanglement when also global and joint measurements were allowed on the \(N - 2\) spins [4]. A lower bound of the localizable entanglement comes from the following theorem [131]

**Theorem 2.3.1** Given a (pure or mixed) state of \(N\) qubits with reduced correlations \(Q^{\alpha,\beta}_{ij} = \langle S^{\alpha}_i S^{\beta}_j \rangle - \langle S^{\alpha}_i \rangle \langle S^{\beta}_j \rangle\) between the spins \(i\) and \(j\) and directions \(\alpha\) and \(\beta\) then there always exist directions in which one can measure the other spins such that this correlation do not decrease, on average.

It then follows that a lower bound to localizable entanglement is fixed by the maximal correlation function between the two parties (one of the various spin-spin correlation functions \(Q^{\alpha,\beta}_{ij}\)).

### 2.4 Entanglement witnesses

It is important to realize that not just the quantification of many-party entanglement is a difficult task; it is an open problem to tell in general, whether a state of \(n\) parties is separable or not although a formal solution of the problem can be written in several forms. It is therefore of great value to have a tool that is able to merely certify if a certain state is entangled. An entanglement witness \(W\) is a Hermitian operator which is able to detect entanglement in a state. The basic idea is that the expectation value of the witness \(W\) for the state \(\rho\) under consideration exceeds certain bounds only when \(\rho\) is entangled. An expectation value of \(W\) within this bound however does not guarantee that the state is separable. Nonetheless, this is a very appealing method also from an

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4These operations in principle need not to be local operations in terms of the multipartite setting of single spins on all the chain.

5The entanglement of assistance is defined as the maximum average entanglement among the pure state realizations of the state under consideration [17].

6It has been argued recently [53, 52] that in order to extend the entanglement of assistance and the localizable entanglement to being an entanglement monotone [133] one should admit also local operations including classical communication on the extracted two spins, this was named entanglement of collaboration.
experimental point of view, since it is sometimes possible to relate the presence of the entanglement to the measurement of few observables.

Simple geometric ideas help to explain the witness operator $W$ at work. Let $T$ be the set of all density matrices and let $E$ and $D$ be the subsets of entangled and separable states, respectively. The convexity of $D$ is a key property for witnessing entanglement\footnote{This is based on the Hahn-Banach separation theorem, stating that given a convex set and a point outside there exists a plane that separates the point from the set.}. The entanglement witness is then an operator defining a hyper-plane which separates a given entangled state from the set of separable states. The main scope of this geometric approach is then to optimize the witness operator [71] or to replace the hyper-plane by a curved manifold, tangent to the set of separable states [56] \footnote{For other geometric aspects of entanglement see [65] [16] [70]}. We have the freedom to choose $W$ such that

$$\text{tr} (\rho_D W) \leq 0$$

for all disentangled states $\rho_D \in D$. Then,

$$\text{tr} (\rho W) > 0$$

implies that $\rho$ is entangled. A caveat is that the concept of a witness is not invariant under local unitary operations (see e.g. [28]).

Entanglement witnesses are a special case of a more general concept, namely that of positive maps. These are injective superoperators on the subset of positive operators. When we now think of superoperators that act non-trivially only on a sub-Hilbert space, then we may ask the question whether a positive map on the subspace is also positive when acting on the whole space. Maps that remain positive also on the extended space are called completely positive maps. The Hermitean time evolution of a density matrix is an example for a completely positive map. Positive but not completely positive maps are important for entanglement theory [61, 64].

**Theorem 2.4.1** A state $\rho_{AB}$ is entangled if and only if a positive map $\Lambda$ exists (not completely positive) such that

$$(\mathbb{1}_A \otimes \Lambda_B) \rho_{AB} < 0.$$ 

For a two dimensional local Hilbert space the situation simplifies considerably in that any positive map $P$ can be written as $P = CP_1 + CP_2 T_B$, where $CP_1$ and $CP_2$ are completely positive maps and $T_B$ is a transposition operation on subspace $B$. This decomposition tells that for a system of two qubits the lack of complete positivity in a positive map is due to a partial transposition. This partial transposition clearly leads to a positive operator if the state is a tensor product of the parts. In fact, also the opposite is true: a state of two qubits $\rho_{AB}$ is separable if and only if $\rho_{AB}^{T_B} \geq 0$ that is, its partial transposition is positive. This is very simple to test and it is known as the Peres-Horodecki criterion [98] [61]. The properties of entangled states under partial transposition lead to a measure of entanglement known as the **negativity**. The negativity $N_{AB}$ of a bipartite state is defined as the absolute value of the sum of the negative eigenvalues of $\rho_{AB}^{T_A}$. The logarithmic negativity is then defined as

$$E_N = \log_2 2(2N_{AB} + 1). \quad (2.17)$$
For bipartite states of two qubits, $\rho^{T_A}_{AB}$ has at most one negative eigenvalue \[110\]. For general multipartite systems and higher local dimension there are entangled states with a positive partial transpose, known as bound entangled states \[1, 62\].

### 2.5 Indistinguishable particles

There is an ongoing debate on which definition of entanglement for indistinguishable particles will be the most useful from a physical point of view. This uncertainty is responsible for the vast variety of quantities studied, when the entanglement of itinerant fermion and boson systems is discussed.

The problem is that for indistinguishable particles the wave function is (anti-) symmetrized and therefore the definition of entangled states as given in the previous Section does not apply. In particular, it does not make sense to consider each individual particle as parts of the partition of the system. Following \[49, 47\] one can address the problem of defining entanglement in an ensemble of indistinguishable particles by seeing if one can attribute to each of the subsystems a complete set of measurable properties, e.g. momenta for free point particles. Quantum states satisfying the above requirement are precisely the (anti-) symmetrization of a product state of (fermions) bosons, and represent the separable states for indistinguishable particles.

There is another crucial difference between the entanglement of (indistinguishable) spin-1/2 particles and that of qubits. Let us consider two fermions on two sites. Whereas the Hilbert space $\mathcal{H}_s$ of a two-site spin lattice has dimension $\dim \mathcal{H}_s = 4$, the Hilbert space $\mathcal{H}_f$ for two fermions on the same lattice has dimension $\dim \mathcal{H}_f = 6$. This is due to the possibility that both fermions, with opposite spins, can be located at the same lattice site. When choosing the following numbering of the states

$$|	ext{1}\rangle = f_1^\dagger |0\rangle =: c_{L,1}^\dagger |0\rangle$$
$$|	ext{2}\rangle = f_2^\dagger |0\rangle =: c_{L,2}^\dagger |0\rangle$$
$$|	ext{3}\rangle = f_3^\dagger |0\rangle =: c_{R,1}^\dagger |0\rangle$$
$$|	ext{4}\rangle = f_4^\dagger |0\rangle =: c_{R,2}^\dagger |0\rangle$$

and the definition $|i,j\rangle = f_i^\dagger f_j^\dagger |0\rangle$, there are Bell states analogous to those occurring for distinguishable particles $(|1, 3\rangle \pm |2, 4\rangle)/\sqrt{2}$ and $(|1, 4\rangle \pm |2, 3\rangle)/\sqrt{2}$. There are however new entangled states, as $(|1, 2\rangle \pm |3, 4\rangle)/\sqrt{2}$, where both fermions take the same position. The local Hilbert space is made of four states labelled by the occupation number and the spin, if singly occupied. The site-entanglement of indistinguishable particles is then defined as the entanglement of the corresponding Fock states. It can be measured e.g. by the local von Neumann entropy. This quantity is the analogue to the one-tangle for qubits, but the local Hilbert space dimension is 4 due to the possibility of having empty and doubly occupied sites. Also the quantum mutual information \[54\] can be defined in this way, quantifying the total amount (classical and quantum) of correlations stored in a given state of a second quantized system.

For spinless fermions a one-to-one mapping to spin-1/2 chains exists in one spatial dimension - the Jordan-Wigner transformation. Due to the non-locality of the Jordan Wigner transformation, quantitative deviations between
the entanglement of spinless fermions and the Jordan-Wigner relative may oc-
cur for distant sites; as far as nearest-neighbor entanglement is considered, both
concepts completely coincide.

Although it is known how the entanglement of indistinguishable particles
can be quantified, as will be seen in the following part, the major part of the li-
terature on second quantized systems considers the site-entanglement described
above or the entanglement of degrees of freedom, singled out from a suitable
set of local quantum numbers (e.g. the spin of the particle at site \(i\)). In both
cases, entanglement measures for distinguishable particles (see Sections 3.4.1
and 3.4.3) can be used.

2.5.1 Two Fermion entanglement

In this paragraph we summarize the distinct features appearing in the quantifica-
tion and classification of Fermion entanglement. Due to the antisymmetry under
particle exchange, there is no Schmidt decomposition for Fermions. Neverthe-
less, a Fermionic analogue to the Schmidt rank, which classifies entanglement
in bipartite systems of distinguishable particles does exist: the so called Slater
rank. A generic state of two-electrons on two lattice sites can be written as

\[
|\omega\rangle := \sum_{i,j=1}^{4} \omega_{i,j} |i, j\rangle
\]

where \(\omega\) is a 4 \(\times\) 4 matrix which can be assumed antisymmetric and normalized
as \(\text{tr} \omega^\dagger \omega = \frac{1}{2}\) (or equivalently \(\text{tr} \omega^* \omega = -\frac{1}{2}\)). Since here the local entities whose
entanglement shall be studied, are the particles, unitary transformations act on
the 4-dimensional single particle Hilbert space. Due to the indistinguishability of
the particles, the transformation must be the same for each of the particles. Gi-
gen a unitary transformation \(U \in \text{SU}(4)\) such that \(f'_j := U j_k f_k\), the transformed state is given by \(|\omega'\rangle\) where \(\omega' := U \omega U^T\). The above unitary transformation
preserves the antisymmetry, and every pure state \(\omega\) of two spin-1/2 particles on
two sites can be transformed into the normal form

\[
\omega_s = \begin{pmatrix}
0 & z_1 & 0 & 0 \\
-z_1 & 0 & 0 & 0 \\
0 & 0 & 0 & z_2 \\
0 & 0 & -z_2 & 0
\end{pmatrix}
\]

In fact, every two-particle state within a \(D\)-dimensional single particle Hilbert
space can be transformed into the normal form

\[
\omega_s = \text{diag}\{Z_1, \ldots, Z_r, Z_0\}
\]

\[
Z_j = \begin{pmatrix}
0 & z_j \\
-z_j & 0
\end{pmatrix}
\]

\[
(Z_0)_{ij} = 0 ; \quad i, j \in \{1, \ldots, D - 2r\}
\]

where \(r\) is then called the Slater rank of the pure Fermion state \([111][112][40]\).
Following the definition in the introduction to this Section, a pure Fermion state
is entangled if and only if its Slater rank is larger than 1.
It is important to notice that the above concept of entanglement only depends on the dimension of the Hilbert space accessible to each of the particles (this includes indistinguishable particles on a single \( D \)-level system).

For electrons on an \( L \)-site lattice the “local” Hilbert space dimension is \( 2^L \), and the question, whether a pure state living in a \( 2^L \)-dimensional single particle Hilbert space has full Slater rank, can be answered by considering the Pfaffian of \( \omega \) \[22\] \[25\] \[85\]

\[
\text{pf}[\omega] := \sum_{\pi \in S_{2L}} \text{sign}(\pi) \prod_{j=1}^{L} \omega_{\pi(2j-1), \pi(2j)}
\]

which is non-zero only if \( \omega \) has full Slater rank \( L \). In the above definition \( S_{2L}^- \) denotes those elements \( \pi \) of the symmetric group \( S_{2L} \) with ordered pairs, i.e. \( \pi(2m-1) < \pi(2m) \) for all \( m \leq L \) and \( \pi(2k-1) < \pi(2m-1) \) for \( k < m \). Notice that relaxing the restriction to \( S_{2L}^- \) just leads to a combinatorial factor of \( 2^L L! \) by virtue of the antisymmetry of \( \omega \) and hence can we write

\[
\text{pf}[\omega] = \frac{1}{2^L L!} \sum_{j_1, \ldots, j_{2L} = 1}^{2L} \varepsilon^{j_1 \ldots j_{2L}} \omega_{j_1, j_2} \omega_{j_3, j_4} \ldots \omega_{j_{2L-1}, j_{2L}}
\]

where \( \varepsilon^{j_1 \ldots j_{2L}} \) is the fully antisymmetric tensor with \( \varepsilon^{1,2,\ldots,2L} = 1 \). There is a simple relation between the Pfaffian and the determinant of an antisymmetric even-dimensional matrix: \( \text{pf}[\omega]^2 = \det[\omega] \).

For the simplest case of two spin-1/2 Fermions on two lattice sites the Pfaffian reads \( \text{pf}[\omega] = \omega_{1,2} \omega_{3,4} - \omega_{1,3} \omega_{2,4} + \omega_{1,4} \omega_{2,3} \). Normalized in order to range in the interval \([0, 1]\) this has been called the Fermionic concurrence \( C[|\omega\rangle] \) \[111\], \[112\], \[40\]

\[
C[|\omega\rangle] = |\langle \tilde{\omega} | \omega \rangle| = 8|\text{pf}[\omega]|
\]

where

\[
\tilde{\omega} := \frac{1}{2} \varepsilon^{ijkl} \omega^*_{k,l}
\]

has been called the dual to \( \omega \). Then, \( |\tilde{\omega}\rangle := D |\omega\rangle \) is the analogue to the conjugated state in \[99\], \[145\], \[123\] leading to the concurrence for qubits. It is important to notice that the Pfaffian in Eq. (2.24) is invariant under the complexification of \( \text{su}(2L) \), since it is the expectation value of an antilinear operator, namely the conjugation \( D \) for the state \( |\omega\rangle \). Since this invariant is a bilinear expression in the state coefficients, its convex roof is readily obtained \[123\] by means of the positive eigenvalues \( \lambda_i^2 \) of the \( 6 \times 6 \) matrix

\[
R = \sqrt{\rho} D \rho D \sqrt{\rho}.
\]

The conjugation \( D \), expressed in the basis \( \{|1, 2\rangle, |1, 3\rangle, |1, 4\rangle, |2, 3\rangle, |2, 4\rangle, |3, 4\rangle\} \) (see Eq. (2.18)), takes the form

\[
\begin{pmatrix}
0 & 0 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 & -1 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 \\
0 & -1 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}
\]

(2.29)
where $C$ is the complex conjugation. Notice that the center part of this matrix (in bold face) is precisely $\sigma_y \otimes \sigma_y$ and indeed corresponds to the Hilbert space of two qubits. The remaining part of the Hilbert space gives rise to an entanglement of different values for the occupation number. This type of entanglement was considered practically useless and has been referred to as the fluffy bunny [142, 128] in the literature.

For a single particle Hilbert space with dimension larger than 4 one encounters similar complications as for two distinguishable particles on a bipartite lattice and local Hilbert space dimension larger than 2, i.e. for two qudits. This is because different classes of entanglement occur, which are characterized by different Slater rank as opposed to their classification by different Schmidt rank for distinguishable particles. The Slater rank can be obtained by looking at Pfaffian minors [85]: if the Slater rank is $r$, all Pfaffian minors of dimension larger than $2r$ are identically zero.

2.5.2 Multipartite Entanglement for Fermions

For indistinguishable particles the only classification available up to now is to check whether or not a pure state has Slater rank one. Eckert et al. formulated two recursive lemmata [40]

**Lemma 2.5.1** A pure $M$-Fermion state has Slater rank one if and only if

$$\sum_{j_1, \ldots, j_M=1}^{2n} \omega_{j_1, \ldots, j_{M-1}} a_{j_M} f^\dagger_{j_1} \cdots f^\dagger_{j_{M-1}} \text{ has Slater rank one or zero for all } a \in \mathbb{C}^{2n}.$$ 

**Lemma 2.5.2** A pure $M$-Fermion state has Slater rank one if and only if

$$\sum_{i_1, \ldots, i_M=1}^{2n} \omega_{i_1, \ldots, i_{M-1}} a_{i_M} a_{i_{M-2}} \cdots a_{i_1} \varepsilon^{i_M-i_{M-1}} a_{i_1} \cdots a_{i_{M-2}} |0\rangle = 0$$

for all $a^1, \ldots, a^{M-2} \in \mathbb{C}^{2n}$ and all $0 \leq \alpha_1 < \cdots < \alpha_{2n-2} \leq 2n$.

They can be summarized as follows: let an $N$-electron state be contracted with $N-2$ arbitrary single electron states encoded in the vectors $a^j$ as $a^j f^\dagger_k |0\rangle$ ($j = 1, \ldots, N-2$ and sum convention) to a two-electron state. Then the Pfaffian of the two-electron state is zero if and only if the original state (and hence all intermediate states in a successive contraction) has Slater rank one. This means that all 4-dimensional Pfaffian minors of $\omega$ are zero.

Instead of the Pfaffian of $\omega$, also the single-particle reduced density matrix can be considered, and its von Neumann entropy as a measure for the quantum entanglement has been analyzed in [72, 95]. It is important to remind that for distinguishable particles the local reduced density matrix has rank one if and only if the original state were a product. This is no longer true for indistinguishable particles. For an $N$-particle pure state with Slater rank one the rank of the single-particle reduced density matrix coincides with the number of particles, $N$. A measure of entanglement is then obtained only after subtraction of the constant value of the von Neumann entropy of a disentangled state. This must be taken into account also for the extension of the measure to mixed states.
2.5.3 “Entanglement of particles”

Entanglement in the presence of superselection rules (SSR) induced by particle conservation has been discussed in Refs. [14, 143, 114, 113]. The main difference in the concept of entanglement of particles [143] from the entanglement of indistinguishable particles as described in the preceding section (but also to that obtained from the reduced density matrix of e.g. spin degrees of freedom of indistinguishable particles) consists in the projection of the Hilbert space onto a subspace of fixed particle numbers for either part of a bipartition of the system. The bipartition is typically chosen to be space-like, as motivated from experimentalists or detectors sitting at distinct positions. E.g. two experimentalists, in order to detect the entanglement between two indistinguishable particles, must have one particle each in their laboratory.

This difference induced by particle number superselection is very subtle and shows up if multiple occupancies occur at single sites for Fermions with some inner degrees of freedom, as the spin. Their contribution is finite for finite discrete lattices and will generally scale to zero in the thermodynamic limit with vanishing lattice spacing. Therefore both concepts of spin entanglement of two distant particles coincide in this limit. Significant differences are to be expected only for finite non-dilute systems. It must be noted that the same restrictions imposed by SSR which change considerably the concept of entanglement quantitatively and qualitatively, on the other hand enable otherwise impossible protocols of quantum information processing [114, 113].

Wiseman and Vaccaro project an $N$-particle state $|\psi_N\rangle$ onto all possible subspaces, where the two parties have a well defined number $(n_A, n_B = N - n_A)$ of particles in their laboratory [143]. Let $|\psi[n_A]\rangle$ be the respective projection, and let $p_{n_A}$ be the weight $\langle \psi[n_A] | \psi[n_A]\rangle / \langle \psi_N | \psi_N\rangle$ of this projection. Then the entanglement of particles $E_p$ is defined as

$$E_p[|\psi_n\rangle] = \sum_n p_n E_M[\psi[n_A]]$$

(2.31)

where $E_M$ is some measure of entanglement for distinguishable particles. Although this certainly represents a definition of entanglement appealing for experimental issues, it is sensitive only to situations, where e.g. the two initially indistinguishable particles eventually are separated and can be examined one-by-one by Alice and Bob. Consequently, “local operations” have been defined in [143] as those performed by Alice and Bob in their laboratory after having measured the number of particles.

Verstraete and Cirac pointed out that the presence of SSR gives rise to a new resource which has to be quantified. They have proposed to replace the quantity $E_p$ with the SSR-entanglement of formation. This is defined as

$$E_f^{(SSR)}[|\psi_N\rangle] = \min_{p_n, \psi_n} \sum_n p_n E_M[\psi_n]$$

where the minimization is performed over all those decomposition of the density matrix where the $|\psi\rangle_n$ are eigenstates of the total number of particles [114, 113].

2.5.4 Entanglement for Bosons

The quantification and classification of boson entanglement is very close in spirit to that of Fermions as described in Section 2.5.1. We therefore will only...
emphasize the marking differences for bosonic entanglement.

In the bosonic case the matrix $\omega$ in Eq. (2.19) is symmetric under permutations of the particle numbers. Consequently, for any two-particle state of indistinguishable bosons, $\omega$ can be diagonalized by means of unitary transformations of the single particle basis. This leads to the Schmidt decomposition for bosons \[40\]. An curious feature distinguishing this case from the entanglement measures of distinguishable particles is that the Schmidt decomposition is not unique. In fact, any two equal Schmidt coefficients admit for a unitary transformation of the two corresponding basis states, such that the superposition of the two doubly occupied states can be written as a symmetrized state of two orthogonal states \[72, 48\]. This is the reason why it is not directly the Schmidt rank, but rather the reduced Schmidt rank - obtained after having removed all double degeneracies of the Schmidt decomposition - that determines whether or not a state is entangled. This non-uniqueness of the Schmidt rank is also responsible for the ambiguity of the von Neumann entropy or other purity measures of the single particle reduced density matrix as an entanglement measure for Bosons \[48\].

With $z_i$ being the Schmidt coefficients with degeneracy $g_i$, the reduced Schmidt rank is at most $\frac{g_i^2}{2} + 2 \{ \frac{g_i}{2} \}$, where $\{ \}$ denotes the non-integer part. As a consequence, a Schmidt rank larger than two implies the presence of entanglement. Schmidt rank 2 with degenerate Schmidt coefficients can be written as a symmetrized product of orthogonal states and consequently is disentangled \[48\]. This feature is also present in the $N$-boson case, where in presence of up to $N$-fold degenerate Schmidt coefficients the corresponding state can be rewritten as a symmetrization of a product.

For bipartite systems $\omega$ has full Schmidt rank if $\det \omega \neq 0$. A Schmidt rank 1 can be verified by the same contraction technique described for the Fermion case in the previous section, where the Pfaffian must be replaced by the determinant. This applies to both the bipartite and the multipartite case \[40\].
Kapitel 3

Entanglement in condensed matter systems

Traditionally many-body systems have been studied by looking for example at their response to external perturbations, various order parameters and excitation spectrum. The study of the ground state of many-body systems with methods developed in quantum information might unveil new insight. In this Section we classify the properties of the ground state of a many-body system according to its entanglement. We first concentrate on spin systems. Spin variables constitute a good example of distinguishable objects, for which the problem of entanglement quantification is most developed. Various aspects mainly of pairwise entanglement will be discussed with some short reference on the properties of bipartite entanglement - as the block entropy - and a comment on the localizable entanglement. Then will we change focus onto itinerant fermion systems.

3.1 Model systems

The model Hamiltonian for a set of localized spins interacting via nearest neighbor exchange coupling in a $d$-dimensional lattice can be written as

$$H(\gamma, \Delta, h^z/J) = J \sum_{\langle i,j \rangle} \left[ \frac{1 + \gamma}{2} S_i^x S_j^x + \frac{1 - \gamma}{2} S_i^y S_j^y + \Delta S_i^z S_j^z \right] - h^z \sum_i S_i^z. \quad (3.1)$$

In the previous expression $i, j$ are lattice points, $\langle \cdot \rangle$ constraints the sum over nearest neighbors and $S_i^\alpha$ ($\alpha = x, y, z$) are spin-1/2 operators. The nomenclature of the various model deriving from Eq. (3.1) is shown in table 3.1. A positive (negative) exchange coupling $J$ favors anti-ferromagnetic (ferromagnetic) ordering in the $xy$-plane. The parameters $\gamma$ and $\Delta$ account for the anisotropy in the exchange coupling, $h$ is the transverse magnetic field.

The ground state of Eq. (3.1) is in general entangled, but for any value of the coupling constants $\gamma$ and $\Delta$, $J > 0$ a value $h_f$ for the magnetic field exists in $d = 1, 2$, where the ground state is factorized \cite{66, 107}. The so called factorizing
| Model | $\gamma$ | $\Delta$ |
|-------|--------|--------|
| XX    | 0      | 0      |
| XY    | $\neq 0$ | 0      |
| XXX   | 0      | 1      |
| XXZ   | 0      | $\neq 0$ |
| XYZ   | $\neq 0$ | $\neq 0$ |
| Ising | 1      | 0      |

Tabelle 3.1: Nomenclature of the various models deriving from Eq. (3.1)

The field $h_f$ is given by

$$h_f = \frac{z}{2} J \sqrt{(1 + \Delta)^2 - (\gamma/2)^2}$$

where $z$ is the coordination number of the lattice. Note that the result for the factorizing field is rigorous irrespective the integrability of the Hamiltonian.

In $d = 1$ the model is exactly solvable in several important cases. In the next two paragraphs we illustrate some of the results obtained for the exactly solvable transverse XY model ($\Delta = 0$ and $0 \leq \gamma \leq 1$). The quantum Ising model is a special case corresponding to $\gamma = 1$ while the (isotropic) XX-model is obtained for $\gamma = 0$. In the isotropic case the model possesses an additional symmetry, resulting in the conservation of the magnetization along the $z$-axis. For any value of the anisotropy the model can be solved exactly \[73, 99, 13\] by a Jordan-Wigner- and a successive Bogoliubov transformation. The Lipkin-Meshkov-Glick model \[74\] which also will appear in the discussion, emerges from the transverse XY-models when the range of spin-exchange, or equivalently the connectivity, is set to infinity.

The properties of the Hamiltonian are governed by the dimensionless coupling constant $\lambda = J/2h$. In the interval $0 < \gamma \leq 1$, the system undergoes a second order quantum phase transition at the critical value $\lambda_c = 1$ \[109, 122\]. The order parameter is the in-plane magnetization (e.g. in $x$-direction: $\langle S_x \rangle$), which is different from zero for $\lambda > 1$. The magnetization along the $z$-direction, $\langle S_z \rangle$, is different from zero for any value of $\lambda$ with singular behavior of its first derivative at the transition. This is reflected also in the singularity present in the second derivative of the ground state energy with respect to $\lambda$. In the whole interval $0 < \gamma \leq 1$ the transition belongs to the Ising universality class. For $\gamma = 0$ the quantum phase transition is of the Berezinskii-Kosterlitz-Thouless type.

### 3.2 Bipartite entanglement and quantum phase transitions

Many scientific investigations have been devoted to the study of entanglement close to quantum phase transition (QPT). In contrast to a standard thermodynamic phase transition, a QPT is a phenomenon that occurs at zero temperature. Its essence consists in a significant qualitative change of the ground state of a model Hamiltonian, which is induced by the change of an external parameter or coupling constant \[109\]. The main idea is that this drastic change of the ground
state should be accompanied by characteristic entanglement patterns. Similar to standard phase transition, also a quantum critical point is characterized by a diverging correlation length $\xi$, which is responsible for the singular behavior of different physical observables. The critical properties in the entanglement we are going to summarize below admit a screening of the qualitative change of the state of the system experiencing a quantum phase transition. In order to avoid possible confusion, it is worth to stress that the study of entanglement close to quantum critical points is not supposed to provide new insight into the scaling theory of quantum phase transitions; rather, it may be useful for a deeper characterization of the ground state wave function of the many-body system undergoing a phase change. In the following, we shine some light on the behavior of the pairwise entanglement, with a subsequent glance at the block entropy.

Pairwise entanglement close to quantum phase transitions was originally analyzed in \[88, 90\] for the quantum XY model in transverse magnetic field in one spatial dimension. For the quantum Ising chain, the concurrence tends to zero for $\lambda \gg 1$ and $\lambda \ll 1$, where the ground state of the system is fully polarized along the $x$-axis and the $z$-axis, respectively. Whereas the full polarization in $z$-direction for small $\lambda$ is guaranteed by the large magnetic field in $z$-direction, this is not the case in the opposite limit for generic values of $\gamma$, and the polarization in this case is an effect due to symmetry breaking. A particularly surprising observation is the short range of the concurrence, in particular at the critical point, notwithstanding the diverging range of two-point spin correlations: the concurrence is zero unless the two sites are at most next-nearest neighbors. This short range in the pairwise entanglement is observed in many different models \[120, 121, 4\], also in higher spatial dimensions. It hence seems to be a generic feature rather than a curious exception. This indicates that pairwise entanglement typically plays a secondary role in Cavour of multipartite entanglement, as far as quantum phase transitions are concerned.

In the Ising case, the concurrence is a smooth function of the coupling with its maximum well separated from the critical point (see the right inset of Fig.3.1). In contrast, the convex roof of the von Neumann entropy shows a pronounced cusp at the critical point \[88\]. The critical properties of the ground state are instead well reflected in the derivatives of the concurrence as a function of $\lambda$. The results for systems of different size (including the thermodynamic limit) are shown in Fig.3.1. For the infinite chain $\partial_\lambda C(1)$ diverges on approaching the critical value as

$$\partial_\lambda C(1) \sim \frac{8}{3\pi^2} \ln |\lambda - \lambda_c|. \quad (3.2)$$

For finite system size, the precursors of the critical behavior can be analyzed by means of finite size scaling. In agreement with the scaling hypothesis, the concurrence depends only on the combination $N^{1/\nu}(\lambda - \lambda_m)$ in the critical region, with critical exponent $\nu = 1$; $\lambda_m$ is here the position of the minimum (see the left inset of Fig.3.1). In the case of log divergence the scaling ansatz has to be adapted for taking care of the critical characteristic log divergence in the

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\[QPTs\] were also studied by looking at quantum fidelity \[32, 149\] or the effect of single bit operations \[51, 50\].
Abbildung 3.1: The change in the ground state wave-function in the critical region is analyzed considering the derivative of the nearest neighbor concurrence as a function of the reduced coupling strength. Different curves correspond to different lattice sizes. On increasing the system size, the minimum gets more pronounced. Also the position of the minimum changes and tends as $N^{-1.86}$ (see the left side inset) towards the critical point where for an infinite system a logarithmic divergence is present. The right hand side inset shows the behavior of the concurrence itself for an infinite system. The maximum is not related to the critical properties of the Ising model. [From [90]]

quantum Ising universality class

\[
\partial_\lambda C(1)(N, \lambda) - \partial_\lambda C(1)(N, \lambda_0) \\
\sim Q[N^{1/\nu} \delta_m(\lambda)] - Q[N^{1/\nu} \delta_m(\lambda_0)] \quad (3.3)
\]

where $\lambda_0$ is some non critical value, $\delta_m(\lambda) = \lambda - \lambda_m$ and $Q(x) \sim Q(\infty) \ln x$ (for large $x$). Similar results have been obtained for the XY models in this universality class [91]. Although the concurrence describes short-range properties, the typical scaling behavior for continuous phase transitions emerges. The analysis of the finite size scaling in the so called period-2 and period-3 chains, where the exchange coupling varies every second and third lattice sites respectively, leads to the same scaling laws in the concurrence [150].

Spontaneous symmetry breaking can influence the entanglement in the ground state. To see this, it is convenient to introduce the thermal ground state in the limit $T \to 0$

\[
\rho_0 = \frac{1}{2} \left( |gs_o\rangle\langle gs_o| + |gs_e\rangle\langle gs_e| \right) = \frac{1}{2} \left( |gs^-\rangle\langle gs^-| + |gs^+\rangle\langle gs^+| \right) . \quad (3.4)
\]

The symmetry broken states $gs^+$ and $gs^-$, which give the correct order parameter of the model, are superpositions of the degenerate parity eigenstates $gs^o$ and $gs^e$. This is the essence of the symmetry breaking in the transverse XY models. Being convex, the concurrence in $gs^\pm$ will be larger than for $gs^{o/e}$ [92]. The opposite is true for the entropy of entanglement (see Ref. [88] for the single spin von Neumann entropy). It was shown, however, that the effect of the spontaneous parity symmetry breaking does not affect the concurrence in the ground
state if it coincides with $C^I$, Eq. (2.13): that is, if the spins are entangled in an anti-ferromagnetic way \[120\]. For the quantum Ising model, the concurrence coincides with $C^I$ for all values of the magnetic field, and therefore, the concurrence is unaffected by the symmetry breaking, the hallmark of the present QPT. For generic anisotropies $\gamma$ instead, also the parallel entanglement $C^{II}$ is observed precisely for magnetic fields larger than the factorizing field \[91\]; this interval includes the critical point $2$. An interpretation of this is that for the Ising universality class, the concurrence is insensitive to the symmetry breaking close to the critical point, and hence won’t play a relevant role in driving this transition. This changes at $\gamma = 0$, where the concurrence indeed shows an infinite range. Below the critical field, the concurrence is enhanced by the parity symmetry breaking \[92\], as shown in Fig. 3.2.

Abbildung 3.2: Left panel: The nearest neighbor concurrence for a chain of 199 sites is shown for three different values $\gamma = 0.3$, 0.5 and 0.7 (circles, squares and diamonds). Full symbols give the results for the even parity ground state. Right panel: Difference of the n.n. concurrence with and without broken parity symmetry as a function of the transverse field. The maximum relative deviation amounts to around 10%; for sufficiently small $h$, it decreases with $\gamma$. Inset: Finite size scaling for $\gamma = 0.7$ and $h/h_f = 0.8$ (diamonds) and limiting value (dashed line).\[From \[92\]\

Several works were devoted to an entanglement analysis close to this factorizing field. The point at which the state of the system becomes separable comes with an exchange of parallel and anti-parallel sector in the ground state concurrence (see Eqs. (2.13) and (2.14)). Furthermore, it is observed that the range of the concurrence diverges close to the factorizing field, in contrast to the typically encountered short range of the concurrence at the critical point. There, the range $R$ is taken as the distance of two qubits, beyond which the concurrence is zero. For the $XY$ model the range was found to diverge close to the factorizing field as \[3\]

$$R \propto \left( \ln \frac{1 - \gamma}{1 + \gamma} \right)^{-1} \ln |\lambda^{-1} - \lambda_f^{-1}|^{-1}$$

(3.5)

The divergence of $R$ suggests, as a consequence of the monogamy of the entanglement \[30 \[89\], that the role of pairwise entanglement is enhanced while approaching the separable point \[103 \[106 \[107\]. Indeed, for the Ising model (i.e.\[2\]To see this, it is enough to realize that a product state of single spin states is a parity eigenstate only if all spins point up or down.
$\gamma = 1$), the ratio $\tau_2/\tau_1 \to 1$ [3], when the magnetic field approaches the factorizing field $h_0$. For $\gamma \neq 1$ and $h_z < h^c < h_c$ it was found that $\tau_2/\tau_1$ monotonically increases with $h_z \to h^c_0$ and that $(\tau_2/\tau_1)|_{h^c_0}$ increases with $\gamma \to 1$. The existence of a factorizing field emerged as a generic feature of spin chains both for short [3, 105, 106] and long ranged interactions [39]; in all these cases the range of the two-site entanglement was observed to diverge.

The section shall be closed with a brief remark concerning the localizable entanglement. From its definition and the fact that it is bound from below by the largest two-point correlation function, it has been presented as a curiosity that an infinite range of entanglement can be present although the correlation functions have finite range. As an example for such behavior the AKLT model, a spin-1 model which exhibits a Haldane gap, has been presented [103]. The infinite range of the localizable entanglement means that by virtue of suitable local transformations, different classes of entanglement can be accumulated on two sites (see also [102] in this context). At the same time, however, also the classical correlations are accumulated and hence would also these localizable classical correlations have an infinite range. The curiosity of having infinite range entanglement but only finite range correlations is hence only due to looking at qualitatively different and not comparable quantities.

### 3.3 Dynamics of entanglement

The interest in studying the properties of entanglement in many-body systems has been directed also to the understanding of its dynamical behavior. Entanglement dynamics has been studied from different perspectives. In a spirit similar to the study of propagation of excitations in condensed matter systems, several works analyzed the propagation of entanglement starting from a given initial state where the entanglement has been created in a given portion of the many-body system. One can imagine for example to initialize a spin chain such that all the spins are pointing upwards except for two neighbor spins which are entangled. Due to the exchange interaction, the initially localized entanglement will spread. This propagation may be ballistic in clean systems or diffusive if some weak disorder is present. Entanglement localization and chaotic behavior could also be observed. An alternative approach is to start with the ground state of a Hamiltonian $H_0$ and then let the Hamiltonian change in time.

Since we are dealing with interacting systems, entanglement can be generated or it can change its characteristics during the dynamical evolution. Besides the interest in their own, attention to these questions has been also motivated by the potential use of one-dimensional spin systems as quantum channels [21]. Another important aspect of entanglement dynamics is the possibility to generate entangled states with certain desired properties by those interactions that are naturally present in a many-body system. This generalizes the setup where a Bell state is created by letting two qubits interact for a fixed time by means of an exchange coupling of the $XX$ type. In the same spirit one can think of generating three-bit entangled GHZ or W states $|W\rangle \sim |100\rangle + |010\rangle + |001\rangle$ - but also other multipartite entangled states - by tailoring the exchange couplings in spin networks or their quantum optical counterpart of atoms in an optical trap potential. Cluster states are a prominent example for genuinely multipartite entangled states, which are generated by Ising type two-spin interactions
from a fully polarized initial state \([58]\).

The most simple situation, which we consider first, is the propagation of entanglement in the one-dimensional \(XX\)-model, i.e. \(\gamma = 0\) and \(\Delta = 0\) in Eq.\(3.1\) \([6, 119]\). This corresponds to free spinless fermions on a discrete lattice. Suppose that the initial state of the chain is

\[
|\Psi_\pm(t = 0)\rangle = \frac{1}{\sqrt{2}}(\sigma_i^x \pm \sigma_j^x)|0,\ldots,0\rangle ,
\]

namely all the spin are in a fully polarized state except the two at positions \(i\) and \(j\), which are prepared in one of the Bell states \(|\psi_\pm\rangle = 2^{-1/2}(|01\rangle \pm |10\rangle)\). In this case the problem has a simple analytical solution. The total magnetization is conserved, and the evolution is confined to the sector with only a single spin pointing up (single-magnon states). The state of a periodic chain at later times is

\[
|\Psi_\pm(t)\rangle = \sum_l w^{(i,j)}_{\pm,l}(t)|l\rangle
\]

with

\[
w^{(i,j)}_{\pm,l}(t) = \frac{1}{\sqrt{2N}} \sum_k \left[ 1 \pm e^{\frac{2\pi ik}{N}(j-i)} \right] e^{\frac{2\pi ik}{N}(j-i)} e^{4iJt \cos \frac{2\pi k}{N}}
\]

In the thermodynamic limit, \(N \rightarrow \infty\), the coefficients can be expressed in terms of Bessel functions \(J_n(x)\)

\[
w^{(i,j)}_{\pm,l}(t) = \frac{1}{\sqrt{2}} \left\{ J_{l-1}(4Jt) \pm (-i)^{j-i} J_{j-1}(4Jt) \right\} .
\]

The concurrence between two sites located at positions \(n\) and \(m\) (initially, only the sites \(i\) and \(j\) were maximally entangled) is given as

\[
C_{n,m}^{(i,j)}(\pm,t) = 2 \left| w^{(i,j)}_{\pm,n}(t) w^{(i,j)*}_{\pm,m}(t) \right| .
\]

and is shown in Fig.\(3.3\) for sites which are symmetrically arranged around the initial position of the Bell state \(|\psi_\pm\rangle\). The Hamiltonian time evolution of the \(XX\) model leads to a propagation of the single flipped spin through the chain. The speed of the propagation is the spin wave velocity in the chain. The information exchange or entanglement propagation over a distance of \(d\) lattice constants approximately takes the time \(t \sim \hbar d/J\). The result is independent of the external field \(h^z\), since the magnetization in \(z\)-direction is a constant of the motion.

This entanglement wave is also the main feature in the behavior of the von Neumann entropy \(S_{n,m}^{(2)}\) of the two sites \((n, m)\) (see Fig.\(3.4\)).

Interesting additional features appear in the quantum \(XY\) model, i.e. for \(\gamma \neq 0\). In this case the magnetization is no longer a constant of the motion (two spins can be flipped simultaneously). The calculations were done analytically \([6]\) resorting on the exact calculation of correlation functions out of equilibrium \([5]\). The most notable difference in the two-site entanglement is an entanglement production from the fully polarized vacuum state. This occurs uniformly along the chain and is superposed onto the entanglement wave discussed before (see
Abbildung 3.3: Concurrence between sites $n = -x, m = x$, symmetrically placed with respect to the sites $i = -1$ and $j = 1$, where the singlet was initially created. [From [6]].

Abbildung 3.4: The two-site entropy $S_{(-n,n+1)}^{(2)}(t)$ for pairs of sites symmetrically displaced with respect to the initial singlet position $(i,j) = (0,1)$. The time is given in units of the exchange coupling $4J$ and the space coordinate $x$ in units of the lattice constant. [From [6]].
Abbildung 3.5: The entanglement wave for the nearest neighbor concurrence is shown here for the Ising model and $\lambda = 0.5$. The initial state is a maximally entangled state of nearest neighbors on top of the fully polarized vacuum state (left) and the ground state (right) respectively. Whereas the propagation velocity is unaffected by the initial state, the entanglement wave reduces the background entanglement in the ground state of the chain (right). [From [6]]

left panel of Fig.3.5). The propagation velocity of the entanglement is almost independent on the anisotropy parameter $\gamma$ and is in well agreement with the sound velocity of the system [118]. What is strongly dependent on $\gamma$ is the damping coefficient of the entanglement wave: as the anisotropy approaches the Ising point $\gamma = 1$, the wave is strongly damped and vanishes already after few time units ($\sim J^{-1}$) at the critical coupling.

The Hamiltonian dynamics primarily generates multipartite entanglement in the chain; this can be seen from the residual tangle [30, 89], which is a measure for entanglement of not only pairs of spins. It is seen from Fig. 3.6 that the major part of the entanglement in the chain is indeed of multipartite origin. This should be expected rather than surprising on the background that multipartite entangled cluster states are created from a fully polarized state by means of a two-spin Ising-type interactions.

3.4 Entanglement in second quantized systems

The theory of entanglement for indistinguishable particles conceptually differs from that for distinguishable constituents; the only factoring state of identical particles is that of bosons all being in the very same state.

The major part of the physical applications still concentrates on those measures applicable for the entanglement encoded in a certain choice of - distinguishable - quantum numbers (see [23]). This analysis captures, of course, a partial aspect of the entanglement encoded in these system; alas, some marking peculiarities due to the indistinguishability of the particles are ignored in this approach. We will report on the established results from these studies and refer to section 2.5 for their relation to fermionic entanglement.
Abbildung 3.6: The residual tangle in case of the Ising model and critical coupling created from the fully polarized vacuum. Multipartite entanglement is clearly dominant over pairwise entanglement. [From [91]]
3.4.1 Free fermions

The site-based entanglement of spin degrees of freedom through the Jordan-Wigner transformation of spinless fermions has been exploited for calculating the concurrence of nearest neighbor sites and the single site von Neumann entropy (see Section 2.5) for the one-dimensional tight-binding model in presence of a chemical potential \[148\]. This model is equivalent to the isotropic $XX$ model in a transverse magnetic field. In this specific case, no double occupancy can occur and the concept of entanglement coincides with that for spins 1/2. It was found that the nearest neighbor concurrence of the ground state at $T = 0$ is maximal at half filling.\(^3\)

The continuous limit of the tight-binding fermion model is the ideal Fermi gas. In this system, the spin entanglement between two distant particles has been studied in \[124\]. There, depending on the dimensionality, the pairwise spin-entanglement of two fermions has been found to decrease with their distance defining a finite range $R$ of the concurrence. The two spin reduced density matrix is

$$
\rho_{12} = \frac{1}{4 - 2f^2} \begin{pmatrix}
1 - f^2 & 0 & 0 & 0 \\
0 & 1 - f^2 & 0 & 0 \\
0 & 0 & 1 - f^2 & 0 \\
0 & 0 & 0 & 1 - f^2
\end{pmatrix}
$$

(3.11)

where $f(x) = d\frac{J_1(x)}{x}$ with $d \in \{2, 3\}$ being the space dimension and $J_1$ the (spherical for $d=3$) Bessel function of the first kind \[124, 87\]. This density matrix is entangled if $f^2 \geq 1/2$. As a consequence, there is spin entanglement for two fermions closer than $d_0 \approx 0.65\frac{\pi}{k_f}$ for $d = 3$ and $d_0 \approx 0.55\frac{\pi}{k_f}$ for $d = 2$ ($k_f$ is the Fermi momentum). A finite temperature tends to diminish slightly the range of pairwise spin entanglement \[87\].

It should not be surprising that non-interacting particles are spin-entangled up to some finite distance. It is true that the ground state and even an arbitrary thermal state of non-interacting fermions has vanishing entanglement among the particles\(^4\) since the corresponding states are (convex combinations of) anti-symmetrized product states. However, disentanglement in momentum space typically leads to entanglement in coordinate space. A monochromatic plane wave of a single particle for example corresponds to a $W$ state, which contains exclusively pairwise entanglement in coordinate space for an arbitrary distance of the sites. Furthermore does a momentum cut-off at $k_f$ correspond to a length scale of the order $\frac{1}{k_f}$.\(^5\)

It is interesting that a fuzzy detection of the particles in coordinate space increases the entanglement detected by the measurement apparatus. In ref. \[26\], the two-position reduced density matrix defined by

$$
\rho_{ss',tt'}^{(2)} = \langle \Psi_{s'}(r')\Psi_{s}(r)\Psi_{s'}(r')\Psi_{s}(r) \rangle
$$

(3.12)

has been calculated for blurred field operators

$$
\Psi_s(r) := \int dr' dp \psi_s(p) D(r - r')e^{ipr'}
$$

(3.13)

\(^3\)Due to particle-hole symmetry, the concurrence is symmetric around half-filling

\(^4\)This statement should not be confused with the non-vanishing \textit{entanglement of particles} \[143\] as observed in \[37\].
where \( D(r - r') = \frac{1}{\sqrt{2\pi\sigma}} \exp \left( -\frac{|r-r'|^2}{2\sigma^2} \right) \) is a Gaussian distribution describing the inaccuracy of the position measurement. This could be understood from the blurred field operators being coherent sums of local field operators; the entanglement measured by the apparatus as described above, is the bipartite entanglement between the two regions of width \( \sigma \) around \( r \) and \( r' \). This entanglement is larger than the average of all pairwise contributions out of it due to the superadditivity of the entropy/negativity. An analysis in [126] for the three fermion spin density matrix revealed that the state carries entanglement within the W-class [38], provided the three particles are in a region with radius of the order of the inverse Fermi momentum; a similar reasoning applies to \( n \) fermions in such a region [126 [77].

### 3.4.2 \( su(2) \) degrees of freedom of interacting fermions

Itinerant systems, where the focus of interest is the entanglement of degrees of freedom forming a representation of \( su(2) \) in terms of the fermionic operators have been also the subject of investigation. This line has been followed in Refs. [148] [117] [125] [45] [126] for analyzing a connection to BCS superconductivity and the phenomenon of \( \eta \)-pairing, a possible scenario for high \( T_c \) superconductivity. Such states appear as eigenstates of the Hubbard model [147] which carry off diagonal long range order. A simplified model of BCS-like pairing for spinless fermions has been studied in [148]. The concurrence of the two qubits represented by the modes \( k \) and \( -k \) has been found to be a monotonically increasing function of the order parameter; it drops to zero significantly before the critical temperature is reached, though.

States with off diagonal long range order by virtue of \( \eta \)-pairing are defined from fermionic operators \( c_{j,\uparrow} \), \( c_{j,\downarrow} \) and the fermionic vacuum \( |0\rangle \) as

\[
\eta_j := c_{j,\uparrow}c_{j,\downarrow} ; \quad \eta := \sum_{j=1}^{L} c_{j,\uparrow}c_{j,\downarrow} \tag{3.14}
\]

\[
|\Psi\rangle = \eta^+ |0\rangle \tag{3.15}
\]

These are symmetric states and consequently, their concurrence vanishes in the thermodynamic limit due to the monogamy property of pairwise entanglement of \( su(2) \) degrees of freedom. Consequently, a connection to the order parameter of off diagonal long range order

\[
O_\eta = \langle \Psi | \eta_j^\dagger \eta_k | \Psi \rangle \tag{3.16}
\]

\[
= \frac{N(L - N)}{L(L-1)} \rightarrow n(1-n)
\]

(with \( N, L \rightarrow \infty \) and fixed filling fraction \( n \)) can not be established, not even for the rescaled concurrence \( C_R \), since

\[
C_R = 2O \left( 1 - \sqrt{\frac{(N-1)(L-N-1)}{N(L-N)}} \right) \rightarrow 1/L
\]

(see also the analysis for the LMG model in Section 3.2). Nevertheless, the state is entangled, as can be seen from the entropy of entanglement and the geometric
measure of entanglement [141]. The latter is tightly connected to the relative entropy [140]. Both have been calculated in Ref. [125] and clearly indicate the presence of multipartite entanglement.

### 3.4.3 Hubbard-type models for interacting fermions

An interesting class of interacting fermion models is that of Hubbard type models. The Hubbard model [42] is defined by the Hamiltonian

\[ H = -t \sum_{\langle ij \rangle} [c_{i,\sigma}^\dagger c_{j,\sigma} + h.c.] + U \sum_i n_{i,\uparrow} n_{i,\downarrow} - \mu N \]  

(3.17)

where \( c_{i,\sigma}, c_{i,\sigma}^\dagger \) are fermionic operators: \( \{ c_{i,\sigma}, c_{j,\sigma'}^\dagger \} = \delta_{i,j} \delta_{\sigma\sigma'} \). The coupling constant \( U \) describes the on-site repulsion, \( t \) is the hopping amplitude and \( \mu \) the chemical potential.

A first study of entanglement in such a system has appeared in [55] for the one-dimensional extended Hubbard model for fermions with spin 1/2. The extension consists in a nearest neighbor density-density coupling \( V \). Due to the conservation of particle number and \( z \)-projection of the spin, the local density matrix of the system takes the simple form

\[ \rho^{(1)} = z \left| 0 \right> \left< 0 | + u^+ \left| \uparrow \right> \left< \uparrow | + u^- \left| \downarrow \right> \left< \downarrow | + w \left| \uparrow \downarrow \right> \left< \uparrow \downarrow | \right. \right. \]  

(3.18)

independent of the site number \( j \) because of translational symmetry. The broken translational invariance in the charge density wave phase has not been taken...
into account in this work. This does not affect the central result but might affect the entropy within the charge density wave phase. Except the superconducting phase, the phase diagram at half filling (for \( \mu = 0 \)) of this model has been nicely reproduced by the contour plot of the local entropy (see Fig. 3.7), where the phase transition lines coincide with its crest. This happens to be an often encountered feature of local entropies - also for spin models - as opposed to the concurrence for pairwise entanglement whose maxima in general appear at a certain distance to quantum critical points and hence are not associated to the quantum phase transition. In view of the monogamy of entanglement this is evidence for dominant multipartite entanglement in the vicinity of quantum phase transitions.

This analysis clearly points out that the local entropy indicates different phase transitions in different ways, essentially depending on whether this quantity is sensitive to its order parameter or not. Due to the \( u(1) \) symmetry of the model, the single site reduced density matrix is a functional of occupation numbers only. These operators cannot, however, describe order parameters of superconductivity or some order parameter of the metal-insulator transition. Indeed, the superconducting phase can be predicted if the entropy of entanglement is calculated for a block of spins, instead of for just a single site \([36]\). A reduced density matrix of at least two sites is necessary for being sensitive to superconducting correlations (see also Ref. \([69]\) for a similar result obtained for the ionic Hubbard model.)

Another model studied with this respect is the so called bond-charge extended Hubbard model, also known as the Hirsch model, which has originally been proposed in the context of high \( T_c \) superconductivity \([60]\). The Hamiltonian is

\[
\mathcal{H} = U \sum_i n_{i,\uparrow} n_{i,\downarrow} - t \sum_i \left[ 1 - x(n_{i,\sigma} + n_{i+1, -\sigma}) \right] c_{i,\sigma}^\dagger c_{i+1,\sigma} + \text{h.c.} \tag{3.19}
\]

For \( x = 0 \) the model \((3.19)\) coincides with the usual Hubbard model \((3.17)\). In phases II and III (see Fig. 3.8) there are superconducting correlations due to \( \eta \)-pairing and hence there is multipartite entanglement, as discussed above \([125]\). For \( x = 1 \), the model is exactly solvable, and the entanglement of the model has been analyzed in Ref. \([9]\). For general \( x \) and \( n = 1 \) see Ref. \([7, 8]\). Besides the local entropy of entanglement \( S_i \), also the negativity \([138]\) and the quantum mutual information \([54]\) \( I_{ij} \) have been used and compared for this analysis. While \( S_i \) measures all (pairwise and multipartite) quantum correlations involving this specific site, the negativity gives a lower bound for the quantum correlation of two specific sites, and the mutual information accounts for pairwise quantum and classical correlations. Therefore, this combination of correlation measures opens the possibility to decide, what type of correlation is relevant at a quantum phase transition. The local entropy is shown in Fig. 3.8. The different phases are discriminated by local occupation numbers; consequently, the entropy \( S_i \) bears the information on all the phase diagram except the insulating line IV. This is seen from the plot of \( \partial_y S_i \) (with \( u = U/t \)) as a function of \( u \) and the filling fraction \( n \). A comparison of first derivatives respect to \( y = n, u \) (depending on the phase transition) of all three correlation measures reveals common singularities for \( \partial_y S_i \) and \( \partial_y I_{ij} \) only for the transitions II-III and II-IV; furthermore, it is found that the range \( R \) of the concurrence diverges\([8]\) at both transitions. These facts allow to judge the transitions II-III and II-IV (at \( n = 1 \)
Abbildung 3.8: **Left panel:** The ground state phase diagram of the Hirsch model at \( x = 1 \). Empty, slashed and full circles indicate the presence of empty, singly and doubly occupied sites, respectively. **Right panel:** Except the insulating line IV, the phase diagram is nicely reproduced by \( \partial_u S_i \). [From [9]]

and arbitrary \( x \) as governed by pairwise entanglement. For the transitions II-I and II-I’ instead, multipartite entanglement is relevant, accompanied by a finite range of the concurrence. A similar behavior was encountered for *non-critical* spin models where the divergence of \( R \) was accompanied by the emergence of a fully factorized ground state. Here, \( R \) diverges close to QPT.

In order to detect the charge transition II-IV at \( n = 1 \) and any \( x \), \( \partial_u S_i \) has been calculated by means of DMRG [7]. Its singularities allowed to accurately determine the charge gap as a function of the bond-charge coupling \( x \).

We finish this selection of results for itinerant fermion systems with the Hubbard model in a magnetic field. Also here, the local entropy \( S_i \) has been looked at in order to analyze its entanglement. As in the examples before, \( S_i \) indicates the second order phase transitions in terms of divergences of its derivatives \( \partial_h S_i \) and \( \partial \mu S_i \), respectively. Indeed, it has been demonstrated that \( \partial_h S_i \) and \( \partial \mu S_i \) can be expressed in terms of spin and charge susceptibilities [6 7]. This bridges explicitly between the standard method in condensed matter physics for studying phase transitions and the approach from quantum information theory.

Summarizing, the body of work developed so far suggests the conclusion that local entropies can detect QPTs in systems of itinerant fermions, particularly if the transition itself is well predicted by a mean field approach for local observables of the model. In the described cases, translational invariance leads to predictions independent of the site, the local entropy is calculated for. In absence of this symmetry, it might prove useful to average over the sites; the resulting measure is then equivalent to the \( Q \)-measure [82].

Though there certainly are transitions with dominant features in the pairwise entanglement, also here the generic case indicates the dominance of multipartite quantum correlations.

### 3.4.4 A remark on entanglement of particles

There is little work which uses measures for indistinguishable particle entanglement (see Section 2.5), particularly regarding the use of the fermionic concurrence, giving account for the possibility of double occupancy (with internal
degree of freedom). The entanglement of particles (see Section 2.5.3) and its difference from the usual spin entanglement has been worked out in [37]; starting with very small systems as two spinless fermions on four lattice sites and the Hubbard dimer, and then for the tight binding model in one spatial dimension, the results are compared with previous results for the spin entanglement in [124].

For the Hubbard dimer (a two-site Hubbard model), the authors compare with the results for the entanglement measured by the local von Neumann entropy without superselection rule for the local particle numbers [148]. Whereas the latter signals decreasing entanglement in the ground state with increasing $U/t$, the entanglement of particles increases [37]. This demonstrates that imposing superselection rules may lead to qualitatively different behavior of the entanglement. Interestingly, an increase with $U/t$ is observed also for the entanglement of modes (without imposing superselection rules)\footnote{For the extended Hubbard dimer, which is defined as the two-site extended Hubbard model, see [35].}

We would like to finish this section with the notice of a recent proposal of an experiment in order to decide whether 'entanglement' merely due to the statistics of the indistinguishable particles can be useful for quantum information processing [27].
Kapitel 4

Multipartite entanglement: quantification and classification

One conclusion from the preceding chapter is that multipartite entanglement plays an important role in condensed matter systems, in particular close to a quantum phase transition. In this chapter we will present a whole variety of quantities that have been proposed for the scope of quantifying and eventually classifying multipartite entanglement.

4.1 A zoo of multipartite entanglement measures

Both the classification of entanglement and its quantification are at a preliminary stage even for distinguishable particles (see however [38, 84, 130, 23, 22, 93, 94, 79, 80] and references therein). This uncertainty is responsible for the vast amount of suggested quantities for the analysis of multipartite entanglement in many-particle systems and in particularly interesting wave functions. It has already been mentioned that several quantities applied in the previous sections are useful as indicators for multipartite entanglement when the whole system is in a pure state; then the cumbersome convex-roof construction is not needed. For non-degenerate ground states of model Hamiltonians, this requirement is met at zero temperature \( T = 0 \). The entropy of entanglement is an example for such a quantity and several works use multipartite measures constructed from and related to it (see e.g. [30, 82, 12, 115, 33, 76]). These measures are of 'collective' nature - in contrast to 'selective' measures - in the sense that they give indication on a global correlation without discerning among the different entanglement classes encoded in the state of the system. The advantage of these measures is that they are easily computed. Their disadvantage is founded in an ambiguity concerning their choice: as soon as at least two different entanglement classes are measured, an infinite variety of inequivalent measures does exist. As an example, infinitely many proposals could be generated from [115, 33, 34, 76] by substituting the standard entropy with another mixedness measure (e.g. the
one-parameter family of Rényi entropies, etc.). Since these new measures will induce a different ordering in the space of entangled states, some results will deviate. The main problem would then consist in extracting the information about different entanglement classes from a vast collection of results. In this context, the authors of Ref. [43, 44] suggest the analysis of a distribution of purities for different bipartitions. If such a distribution is sufficiently regular, its average and variance might prove characteristic for the global entanglement in the system. The application of this analysis to the one-dimensional quantum Ising model in a transverse field revealed a well behaved distribution function, whose average and second moment are good indicators of the quantum phase transition [31]: at the quantum critical point both the average and the standard deviation exhibit a peak that becomes more pronounced as the number of qubits is increased.

Another pragmatic way of quantifying entanglement in a collective way is represented by the geometric measure of entanglement [141]. It quantifies the entanglement of a (pure) state through the minimal distance of the state from the set of (pure) product states [127, 141]

$$E_g(\Psi) = -\log_2 \max_\Phi |\langle \Psi | \Phi \rangle|^2$$

(4.1)

where the maximum is on all product states $\Phi$. As discussed in detail in [141], the previous definition is an entanglement monotone. It is zero for separable states and rises up to unity for e.g. the maximally entangled n-particle GHZ states. The difficult task in its evaluation is the maximization over all possible separable states and of course the convex roof extension to mixed states.

A different approach was pursued in [57] (see also [116]) where different bounds on the average energy of a given system are obtained for different types of n-particle quantum correlated states. A violation of these bounds then implies the presence of multipartite entanglement in the system. The starting point of Gühne et al. are the n-separability and k-producibility which admit to discriminate particular types of n-particle correlations present in the system. A pure state $|\psi\rangle$ of a quantum systems of N parties is said to be n-separable if it is possible to find a partition of the system for which $|\psi\rangle = |\phi_1\rangle|\phi_2\rangle \cdots |\phi_n\rangle$. A pure state $|\psi\rangle$ can be produced by k-party entanglement (i.e. it is k-producible) if we can write $|\psi\rangle = |\phi_1\rangle|\phi_2\rangle \cdots |\phi_m\rangle$ where the $|\phi_i\rangle$ are states of maximally k parties; by definition $m \geq N/k$. It implies that it is sufficient to generate specific k-party entanglement to construct the desired state. Both these indicators for multipartite entanglement are collective, since they are based on the factorizability of a given many particle state into smaller parts. k-separability and k-producibility both can not discriminate the different k-particle entanglement classes (as e.g. the k-particle W-states and different k-particle graph states [58], like the GHZ state).

Another approach pursued is the generalization of the celebrated concurrence. For the quantification of pairwise entanglement in higher dimensional local Hilbert spaces, the concept of concurrence vectors has been formulated [10, 11] besides the I-concurrence [108]; the length of the concurrence vector has proved equivalent to the I-concurrence [146]. Also for multipartite systems of qubits the concurrence vector concept has been proposed [2]. In the multipartite setting however this means to apply the pure state concurrence formula to a mixed two-site reduced density matrix. It will coincide with the true con-
currence if and only if the eigenbasis of the density matrices accidentally are an optimal decomposition. Therefore, the concurrence vector in this case is not a vector whose entries are the concurrences, and it is at least not obvious whether this proposal is an entanglement monotone.

The \( n \)-tangle is a straightforward extension of the concurrence to multipartite states as the overlap of the state with its time-reversed \[^{144}\] . It vanishes identically for an odd number of qubits, but an entanglement monotone is obtained for an even number of qubits. Due to its factorizing structure, it detects products of even-site entangled states in addition to certain genuine multipartite entangled states: it detects the multipartite GHZ or cat state, but not for example the four qubit cluster state. Therefore, also the \( n \)-tangle is a collective measure.

### 4.2 Measures for genuine multipartite entanglement

The counterpart to collective entanglement measures are selective measures for each different multipartite entanglement class separately. A first multipartite example beyond pairwise qubit entanglement has been derived from the concurrence and the (one-)tangle: the 3-tangle \[^{30}\] . It is a measure for genuine tripartite entanglement that discriminates also from pairwise entanglement distributed all over the chain, as is the case for the \( W \) state \( |W\rangle \sim |100\rangle + |010\rangle + |001\rangle \). The 3-tangle coincides with the 3-dimensional hyperdeterminant for two-dimensional local vector spaces \[^{83}\] , i.e. a generalized determinant form for 3x2 matrices over \( \mathbb{C} \). It originated the insight that \( SL(2, \mathbb{C}) \) invariance rather than \( SU(2) \) invariance leads to a classification of genuine multipartite entanglement: the 3-tangle is indeed the only \( SL(2, \mathbb{C}) \)^{⊗3} invariant, and only a single entanglement class with respect to SLOCC \[^{38}\] does exists. The task of finding SLOCC-class selective measures of qubit entanglement hence is reduced to finding local \( SL(2, \mathbb{C}) \) invariant operators, from which global \( SL(2, \mathbb{C})^{⊗n} \) invariants can be constructed.

The invariance group should be extended to including the symmetric group \( S_q \) for \( q \)-partite systems\[^{93}\] . The genuine multipartite entangled states belong to the non-zero SLOCC class\[^{2}\].

There are standard formalisms in the well developed field of invariant theory for the construction of all \( SL(2, \mathbb{C})^{⊗n} \) invariants (see Ref. \[^{22}\] and references therein, but also Ref. \[^{129}\] for the contraction method with the invariant tensor, which for qubits or spins-1/2 is \( i\sigma_y \)). However, the construction of a complete set is very cumbersome already for five qubits \[^{74}\] and the so constructed invariants will typically be non-zero also for certain factorizing states, and consequently will they be collective measures. Furthermore would we desire to walk in the steps of Wootters’ concurrence and to write the invariants as expectation values of some tangle operator. The minimal requirement would then be that the measure of a somehow factorizing state should be zero. Interestingly, it seems that

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1 This amounts to including the permutation of qubits to the realm of “local” operations; this bigger symmetry group has been termed \( SL_{loc}^n \) in Ref. \[^{29}\].

2 The complementary zero SLOCC class is made of those states that vanish after - maybe infinitely many - suitable \( SL(2, \mathbb{C}) \) operations; the non-zero SLOCC class is the complement of the zero SLOCC class.
this ‘minimal’ requirement already implies the necessary invariance, at least for qubits \[93\, 94\].

The special case of factorization into a single qubit and the remaining (n-1) qubits leads to the central quality of the local operators we are searching for: its expectation value should vanish for all single qubit states \(|\psi\rangle\langle\psi|\) 

\[
\langle\psi| \mathcal{O} |\psi\rangle \equiv 0 \quad (4.2)
\]

Such an operator can impossibly be linear, and antilinear operators have to be studied \[93\]. The unique antilinear operator satisfying Eq. (4.2) is \(\sigma_y \mathcal{C}\), as used for the definition of the pure state concurrence, where \(\mathcal{C}\) is the complex conjugation in the eigenbasis of \(\sigma_z\). It is suggested from the described shortcomings of the n-tangle as a measure for genuine multipartite entanglement measure \[144\] that at least one further operator besides \(\sigma_y\) will be needed. Such an additional operator is found when the requirement (4.2) is extended to the two-fold copy of single qubit states 

\[
\langle\psi| \bullet \langle\psi| \mathcal{O} |\psi\rangle \bullet |\psi\rangle \equiv 0 \quad (4.3)
\]

The requirement to being trace-norm orthogonal to \(\sigma_y \bullet \sigma_y \mathcal{C}\) leads to the unique (up to normalization) operator 

\[
\sum_{\mu=0}^{3} g_{\mu} \sigma_{\mu} \bullet \sigma_{\mu} \mathcal{C} =: \sigma_{\mu} \bullet \sigma^{\mu} \mathcal{C} \quad (4.4)
\]

where \(g_{\mu} : (g_0, g_1, g_2, g_3) = (-1, 1, 0, 1)\) and \(\sigma_0 = 1_2\). Both antilinear operators are invariant under \(SL(2, \mathbb{C})\) operations on the qubit.

One possible way of expressing the 3-tangle in terms of the above mentioned pair of antilinear operators is 

\[
\tau_3[\psi] = \frac{1}{3} \langle\psi^*| \bullet \langle\psi^*| \sigma_{\mu} \otimes \sigma_{\nu} \otimes \sigma_{\lambda} \otimes \sigma^{\mu} \otimes \sigma^{\nu} \otimes \sigma^{\lambda} |\psi\rangle \bullet |\psi\rangle . \quad (4.5)
\]

This form has the minimal possible multi-linearity and it is evidently permutation invariant. Unfortunately, the convex roof construction presented in Refs. \[145\, 123\] for bilinear quantities can not in general be extended to higher multi-linearity. This is very much related to the absence of a tilde-orthogonal basis \[145\] that exists for bi-antilinear constructions (see \[123\]).

A first success in direction of an understanding of convex roofs for multipartite entanglement measures is the analytic convex roof construction found for rank two-mixtures of translational invariant \(GHZ\) and orthogonal \(W\) states \[75\].

The result is best expressed in the Bloch sphere of both orthogonal states (left panel of Fig. 4.1). The right panel of Fig. 4.1 shows the convex roofs of the three entanglement measures tangle(solid line), concurrence (dashed line) and 3-tangle (dotted line), which enter the monogamy relation of Coffman \textit{et al}.

The curious result is that an interval with vanishing concurrence and 3-tangle appears, whereas the tangle is always positive. On the background that only two classes of entanglement exist for three qubits \[38\], this result might appear contradictory at first sight. That this is not the case, is due to a subtlety of convex roof measures, when different entanglement classes are considered (here the concurrence - pairwise - and the 3-tangle). The explanation is that the optimal decompositions leading to the respective convex roofs, will in general not be
compatible, in the sense that both will not emerge from a single optimal decomposition of the whole density matrix. The physical interpretation of this curious finding is very simple: in the interval of vanishing concurrence and 3-tangle, the density matrix can be built from pure states that have either concurrence or 3-tangle (or both).

With the two independent local $SL(2,\mathbb{C})$-invariant operators (combs) $4.2$ and $4.3$ at hand, entanglement measures for genuine multipartite entanglement can now be constructed for an arbitrary number of qubits. The astonishing news from the four qubit case is that three inequivalent measures for SLOCC entanglement classes do exist $93$.

\[ F_1^{(4)} = (\sigma_\mu \sigma_\nu \sigma_\rho \sigma_\sigma) \cdot (\sigma_\mu \sigma_\nu \sigma_\lambda \sigma_\sigma) \cdot (\sigma_\rho \sigma_\lambda \sigma_\omega \sigma_\omega) \]  
\[ F_2^{(4)} = S((\sigma_\mu \sigma_\nu \sigma_\rho \sigma_\omega) \cdot (\sigma_\mu \sigma_\nu \sigma_\lambda \sigma_\omega) \cdot (\sigma_\rho \sigma_\lambda \sigma_\sigma \sigma_\lambda) \cdot (\sigma_\rho \sigma_\lambda \sigma_\omega \sigma_\sigma) \]  
\[ F_3^{(4)} = \frac{1}{2} (\sigma_\mu \sigma_\nu \sigma_\rho \sigma_\rho) \cdot (\sigma_\mu \sigma_\nu \sigma_\lambda \sigma_\omega) \cdot (\sigma_\rho \sigma_\lambda \sigma_\sigma \sigma_\omega) \cdot (\sigma_\rho \sigma_\lambda \sigma_\omega \sigma_\sigma) \] 

where $S$ indicates the symmetrization with respect to the permutation group $S_4$ on four qubits. This leads to seven inequivalent representatives of SLOCC entanglement classes for four qubits. These include the GHZ state $4.9$, the celebrated cluster state $4.10$ (three states connected by means of $S_4$ permutations) and a third state $4.11$, which in contrast to the former two has non-zero

\[ p_{1} \quad p_{0} \]

\[ 0 \quad 0.2 \quad 0.4 \quad 0.6 \quad 0.8 \quad 1 \]

Abbildung 4.1: **Left panel:** Bloch sphere for the two-dimensional space spanned by the GHZ state and the W state. The simplex $S_0$ contains all states with zero three-tangle. The leaves between $p_0$ and $p_1$ represent sets of constant three-tangle, and in the simplex $S_1$ the three-tangle is affine. The corners of the simplices constitute the optimal decomposition. **Right panel:** Plot of the convex roofs of the tangle (solid line), concurrence (dashed line) and 3-tangle (dotted line). There is an interval with entangled states without concurrence or three-tangle. [From $[75]$]
4-qubit hyperdeterminant.

\[ | \Phi_2 \rangle = \frac{1}{\sqrt{2}} ( | 0000 \rangle + | 1111 \rangle ) \quad (4.9) \]
\[ | \Phi_4 \rangle = \frac{1}{2} ( | 1111 \rangle + | 1100 \rangle + | 0010 \rangle + | 0001 \rangle ) \quad (4.10) \]
\[ | \Phi_5 \rangle = \frac{1}{\sqrt{6}} ( \sqrt{2} | 1111 \rangle + | 1000 \rangle + | 0100 \rangle + | 0010 \rangle + | 0001 \rangle ) \quad (4.11) \]

Furthermore, representatives of \( q - 1 \) inequivalent non-zero SLOCC classes \([38, 129]\) are known for \( q \)-qubits \([94]\). Explicit measures for up to six qubits and a prescription how general \( q \)-qubit entanglement measures are constructed have been given in Ref. \([94]\); their characteristics on \( q - 1 \) maximally entangled states demonstrates that the states belong to different non-zero SLOCC classes (see table 4.2).

Tabelle 4.1: Filter values for maximally entangled states; the length is the number of Fock-elements in their canonical form. The 5- and 6-qubit entanglement measures are explicitly given in Ref. \([94]\) together with the maximally entangled states they have been evaluated on here.

| length | \( | \mathcal{F}_1^{(4)} | \) | \( | \mathcal{F}_2^{(4)} | \) | \( | \mathcal{F}_3^{(4)} | \) | \( | \mathcal{F}_1^{(5)} | \) | \( | \mathcal{F}_2^{(5)} | \) | \( | \mathcal{F}_3^{(5)} | \) | \( | \mathcal{F}_1^{(6)} | \) | \( | \mathcal{F}_2^{(6)} | \) |
|--------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| 2      | 1               | 1               | 1               | 1               | 1               | 1               | 1               | 1               |
| 4      | 0               | \( \frac{1}{3} \) | 1               | 0               | 0               | 0               | 1               | 0               |
| 5      | \( \frac{8}{9} \) | 0               | 0               | 0               | \( \frac{2^6}{3^2} \) | 0               | 0               | 0               |
| 6      | X               | X               | X               | \( \frac{3\sqrt{3}}{32} \) | 0               | 0               | 0               | 0               |
| 7      | X               | X               | X               | X               | X               | X               | X               | 0               |

Summarizing, a method has been constructed that permits to construct measures for genuine multipartite entanglement, i.e. for the non-zero SLOCC class of entangled states. Eventually necessary symmetrization with respect to the corresponding symmetric group leads to generators of the ideal of \( SL^* \)-invariants \([29]\) that vanish on arbitrary product states. The generators of this ideal can also be constructed from the invariants known from invariant theory \([78, 29, 79]\). It would be highly desirable to bridge between both approaches. For four qubits, this bridge has already been established by the author in collaboration with D. Ž. Doković to the extent that the three 4-qubit entanglement measures have been expressed in terms of three generators of that ideal but constructed from the standard invariants from \([78, 29]\). The results will be presented in a forthcoming publication. \(^4\)

\(^4\)Note added after the habilitation procedure: this work is now available on the arXiv:0804.1661
4.3 Experimental access to genuine multipartite entanglement

The invariants under local $SL(2, \mathbb{C})$ operations are most naturally expressed in terms of expectation values of antilinear operators. However, in the laboratory physical observables are measured, which are linear operators. So, unless the experiment is performed with quantum states with real coefficients only, a translation of the above multipartite entanglement measures into spin correlation functions will be necessary. Such a one-to-one translation indeed exists. In order to see how the modulus of antilinear expectation values can be transported into linear expectation values, we write

$$\langle \psi | (\hat{O} \otimes \ldots) | \psi^* \rangle \ldots \langle \psi^* | (\hat{O} \otimes \ldots) | \psi \rangle \ldots$$

$$= \langle \psi | \cdot \langle \psi^* | \cdot \ldots [\hat{O} \cdot \hat{O} \cdot \ldots] \otimes \ldots | \psi^* \rangle \cdot | \psi \rangle \cdot \ldots$$

(4.12)

$$= \langle \psi | \cdot \langle \psi^* | \cdot \ldots [(\hat{O} \cdot \hat{O} \prod \mathcal{P}_{i,i'}) \ldots] \otimes \ldots | \psi^* \rangle \cdot | \psi \rangle \cdot \ldots$$

where $\mathcal{P}_{i,i'}$ is the permutation operator acting on the corresponding different copies of the same qubit and the product extends over all qubits and various copies such that exclusively linear expectation values occur. As a consequence, the linear operator corresponding to an antilinear operator $\mathcal{O}$ is then

$$\mathfrak{L}[\mathcal{O}] := (\mathbb{I} \cdot \mathcal{C})(\mathcal{O} \cdot \mathcal{O}) \mathcal{P}$$

(4.13)

It is clear that the transformation in the opposite direction works the same way. In particular we find

$$\mathfrak{L}[\sigma_y] = M_{\mu\nu} \sigma_\mu \cdot \sigma_\nu$$

(4.14)

$$M_{\mu\nu} = \text{diag}\{1, -1, -1, -1\}$$

(4.15)

It is worth noticing that $M_{\mu\nu}$ is precisely the Minkowski metric.

$$\mathfrak{L}[\sigma_{\mu} \cdot \sigma^\mu] = \frac{1}{4} \mathcal{G}_{\kappa\lambda\mu\nu} \sigma_\kappa \cdot \sigma_\lambda \cdot \sigma_\mu \cdot \sigma_\nu$$

(4.16)

$$\mathcal{G}_{\kappa\lambda\mu\nu} = \delta_{\lambda+\kappa,3} \delta_{\mu+\nu,3} \mathcal{H}_{\mu\nu} + \delta_{\kappa\mu} \delta_{\lambda\nu} \mathcal{J}_{\mu\nu}$$

(4.17)

$$\mathcal{H} = \begin{pmatrix} -2 & 0 & 0 & -2 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -2 & 0 & 0 & -2 \end{pmatrix}, \quad \mathcal{J} = \begin{pmatrix} 2 & 0 & 0 & 2 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 2 & 0 & 0 & 2 \end{pmatrix}$$

(4.18)

This is a straightforward prescription for expressing the genuine multipartite entanglement measures presented in Ref. [93, 94] in terms of expectation values of linear operators. The details of this transcription including an analysis of weakly mixed states will be presented in a forthcoming publication.

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$^5\mathcal{P} = \frac{1}{2} \sigma_\mu \cdot \sigma_\mu$, using Einstein sum convention
In conclusion, quantum entanglement is a fascinating phenomenon that naturally occurs in the eigenstates of interacting Hamiltonians. It is certainly the interpretation of this entanglement as a resource for quantum information processing that nowadays is mainly responsible for its growing relevance and consideration in e.g. condensed matter physics. Nevertheless did measures for certain classes of entanglement also prove to be useful tools for the indication of quantum phase transitions if the corresponding measure (e.g. some entanglement entropy) incorporates the relevant order parameter. Though there is only a single class-selective entanglement measure we can compute for mixed states, namely the concurrence for pairwise entanglement of qubits, the Coffman-Kundu-Wootters relation makes the local von Neumann entropy to an implicit indicator of multipartite entanglement. The analysis of ground state entanglement of many model Hamiltonians gives strong support to the conclusion that multipartite entanglement becomes dominant in quantum Hamiltonians close to their critical point. But it is also rather multipartite than only pairwise entanglement, that is created by Hamiltonian evolution from disentangled initial states. A deeper analysis is needed here in particular in the direction of more conclusive measures rather than analyzing more and more different Hamiltonians with always the same canonical set of measures. On the other hand, since the presence of multipartite entanglement seems to be the generic case rather than the exception, it might be the weakly or even disentangled states, as for the factorizing field in spin chains, which are the precursors of drastic changes and complex phenomena. In any case must the understanding of entanglement and its subdivision into distinct SLOCC classes be improved substantially before a possible connection between entanglement and quantum phase transitions can be established. A step into this direction is to realize that the relevant symmetry group for entanglement classification is the local $SL(2,\mathbb{C})$, including the permutation group of the qubits, and that entanglement monotones for this invariance group can be built from local invariant and antilinear operators with zero expectation values on all the local Hilbert space - combs. Two such operators have been found recently for qubits. They permit the construction of a complete set of measures for genuine multipartite entanglement provably up to 4 qubit systems. The main achievement lies in that the combs admit a straightforward construction of the ideal of $SL(2,\mathbb{C})^\otimes N$-invariants whose elements vanish on all product states and for arbitrary number of qubits $N$; this is a problem which already for five qubits
creates severe difficulties for standard methods from invariant theory, where it seems hopeless to handle them for systems larger than this. A one-to-one correspondence of the antilinear invariants to correlation function finally even gives a prescription for the laboratory in order to extract these quantities from spin correlation functions. Yet, this is rather the very beginning of research in this direction, since there is little understanding of even very elementary questions. Although a set of maximally entangled states is given for an arbitrary number of qubits, the ambiguity of such a set is an issue: it is not clear from the beginning, whether a complete set of maximally entangled states can possibly be constructed from them as elements of kind of a basis for such states. A characterization of maximally entangled states might be thinkable in terms of the analogue of a tilde-orthogonal basis (see [143]). Completeness of the ideal is another big issue which would have an important impact also in the field of invariant theory. A further major challenge consists in the extension of the pure state measures to mixed states, which at the end is necessary in order to express the entanglement measure in terms of correlation functions of a practically infinitely large condensed matter system. Also here an important step forward has been done on the mixture of three qubit GHZ and W states, but the ultimate goal would be an analytic procedure for the convex roof extension along the lines of the concurrence. Already now the accumulated knowledge about optimal decompositions is of substantial help for numerical procedures and leads to nontrivial lower bounds for multipartite entanglement in mixed states, but the major part of the puzzle pieces is yet to be found. A consequent extension of the method of combs would consist in their identification for local Hilbert space dimension larger than two. Here the problem is more complex already at the starting point, because there are no bi-antilinear $SL(2S + 1, \mathbb{C})$ invariant combs for spin $S > \frac{1}{2}$. Last but not least we mention that once, genuine multipartite entanglement measures are known, they should be used for testing and analyzing alternative approaches to the detection of entanglement. Witnesses are one relevant example of a complementary approach, which is motivated from the question for separability of a mixed quantum state rather than from the classification of entanglement. It might be just their complementarity bearing the key towards many open questions in the theory of entanglement.
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